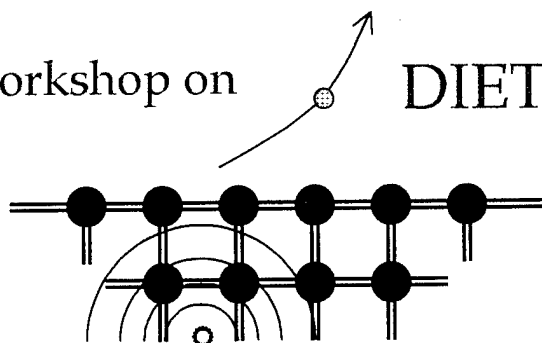


8th International Workshop on
Desorption
Induced by
Electronic
Transitions



DIET 8

San Alfonso / Long Branch / New Jersey / USA

27 September – 1 October 1999

Program and Abstracts

THE STATE UNIVERSITY OF NEW JERSEY

RUTGERS

Laboratory for Surface Modification

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13. ABSTRACT (Maximum 200 words) The primary purpose of the DIET-8 workshop was to assemble the world's authorities in electronically-induced surface processes (mainly, but not restricted to, desorption). The field of electronic excitations on surfaces and the subsequent atomic and molecular changes induced by these excitations has been expanding greatly, especially in the areas of atomically-resolved DIET processes, femtosecond dynamics, and photochemistry. Applications are myriad, including semiconductor processing, beam damage in quantitative surface analysis, photocatalysis, and surface chemistry in interplanetary space. This workshop thus served as a very important forum to discuss, analyze, and assess recent progress in both the theoretical understanding of these complicated phenomena and the latest experimental results. The workshop was attended by 70 attendees from 11 countries; 42 oral presentations and 19 posters were presented. This Proceedings volume contains 39 papers selected from the presentations at the workshop, following regular refereeing procedures of Surface Science.			
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DIET 8

The Eighth International Workshop on Desorption Induced by Electronic Transitions, DIET-8, builds on the tradition of earlier meetings in the DIET series (held at 2 1/2 year intervals). The focus is on desorption and dynamical processes at surfaces, initiated by photon, electron or ion bombardment.

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Frank M. Zimmermann, *Rutgers University*
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Rutgers Laboratory for Surface Modification

DIET Workshops

DIET 1, 1982, Williamsburg Virginia, USA	DIET 5, 1992, Taos, New Mexico, USA
DIET 2, 1984, Schloss Elmau, Germany	DIET 6, 1994, Krakow, Poland
DIET 3, 1987, Shelter Island, New York, USA	DIET 7, 1997, Ambleside, UK
DIET 4, 1989, Gloggnitz, Austria	DIET 8, 1999, Long Branch, New Jersey, USA

MONDAY SEPTEMBER 27

12:00 - 6:00 p.m. -Arrive at San Alfonso; Check-in; Registration

6:00 p.m. - DINNER -

7:30 p.m. - WELCOMING RECEPTION -

TUESDAY SEPTEMBER 28

TUESDAY MORNING

8:00 - BREAKFAST -

SESSION TuM1 - Chair, Frank M. Zimmermann

8:50 Opening Remarks, T. E. Madey, *Rutgers University*

9:00 INVITED - DIET-Related Processes in Atomic Manipulation
G. Dujardin, *Université Paris-Sud, Orsay*

9:40 Vibrational Excitation and Electron Induced Dissociation by the STM:
Pyridine and Benzene on Cu(001)
L. J. Lauhon** and W. Ho, *Cornell University*

10:00 Dynamics of Photodissociation of Adsorbed Nitrites on Ag(111):
Rotationally Resolved Resonance Enhanced Multiphoton Ionization Time-
of-Flight (REMPI-TOF) NO Spectra
Wei Zhao**, Chulhoon Kim, and J. Mike White, *The University of Texas at Austin*

10:20 - COFFEE BREAK -

SESSION TuM2 - Chair, Roger Azria

10:50 INVITED - Recent Progress in the Investigation of Core Hole-Induced PSD
From Adsorbates: Excitation Site Dependent Bond Breaking, and Charge
Rearrangement
P. Feulner, *Technische Universität München*

11:30 Photodesorption of Molecular Nitrogen from Pt(111)
C. French, B.C. Haynie, A. Solodukhin, I. Harrison, and R. Zehr**, *University of Virginia*

12:00 - LUNCH -

** Competing for Student Award

TUESDAY AFTERNOON

SESSION TuA1 - Chair, Dietrich Menzel

- 1:20 **INVITED - Stimulated Desorption by Electron Standing Waves**
M. T. Sieger, *Pacific Northwest National Laboratory*
- 2:00 **Discriminating Time and Angles: TOF-ESDIAD Studies of Interactions between Particles Adsorbed on a Single Crystal Metal Surface**
Dan Mocuta^{**}, Joachim Ahner, and John T. Yates, Jr., *University of Pittsburgh*
- 2:20 **Electron Beam Induced Degradation of Zinc Sulfide-Based Phosphors**
B. L. Abrams^{**}, W. Roos, and P. H. Holloway, *University of Florida*
H. C. Swart, *University of the Orange Free State*
- 2:40 **Electronic Sputtering of Condensed Gas Solids**
E. M. Bringa^{**} and R. E. Johnson, *University of Virginia*
- 3:00 - COFFEE BREAK -

SESSION TuA2 - Chair, David Langreth

- 3:30 **INVITED - Molecular Desorption from Surfaces - A Testing Ground for Dissipative Quantum Dynamics**
Shiwu Gao, *Chalmers University*
- 4:10 **A First Principles Study of Laser Induced Desorption: Ab Initio and Wave Packet Calculations**
T. Klüner, S. Thiel, and H.-J. Freund, *Fritz-Haber-Institut, Berlin*
V. Staemmler, *Ruhr-Universität Bochum*
- 4:30 **Dissociation of an Adsorbate Surface Bond by Direct Optical Excitation: H-Si(100)**
T. Vondrak and X.-Y. Zhu, *University of Minnesota*
- 4:50 **Photodesorption and Electronic Relaxation**
G. Comtet, L. Hellner, G. Dujardin, and V. Bellanger, *Universitaire Paris-Sud*
- 5:10 **Photodissociation of CH₃I/Cu(110): Surface Effects in Dissociation Pathways**
C.C. Johnson and E.T. Jensen, *University of Northern British Columbia*
- 6:00 - DINNER -
- 7:30 - 9:30 POSTER SESSION

^{**}Competing for Student Award

WEDNESDAY SEPTEMBER 29

WEDNESDAY MORNING

8:00

- BREAKFAST -

SESSION WeM1 - Chair, Norman Tolk

9:00

INVITED - Adsorbate Photochemistry and Electron Chemistry
John C. Polanyi, *University of Toronto*

9:40

Photoexcited Electrons and Induced Vibrational Pre-Desorption on a Metal Surface
Pui-Teng Howe and Hai-Lung Dai, *University of Pennsylvania*

10:00

Energy-Resolved Angular Distributions for Photoinduced DEA to Methyl Bromide on GaAs(100): Photochemically-Induced Surface Reconstruction and Evidence for Site Specificity
K. A. Khan, N. Camillone III, J. Yarmoff, and R. M. Osgood, Jr., *Columbia University*

10:20

- COFFEE BREAK -

SESSION WeM2 - Chair, Hai-Lung Dai

10:50

Surface Dynamics Using Pulsed Electron Beams
Ally S.Y. Chan and Robert G. Jones, *University of Nottingham*

11:10

Selectivity of Bond-Breaking in Electron-Induced Dissociation (EID) of Hydrocarbon Films on Au Surfaces
D. Semin and B. E. Koel, *University of Southern California*

11:30

Photoinduced Hot Electron Transfer to Self-Assembled Monolayers of Molecular Quantum Dots on Metal Surfaces
T. Vondrak and X.-Y. Zhu, *University of Minnesota*

12:00

- LUNCH -

WEDNESDAY AFTERNOON

- OUTING AND BANQUET -

1:15

Buses depart San Alfonso for Ellis Island and Statue of Liberty

6:30

Banquet at Molly Pitcher Inn, Red Bank, NJ

THURSDAY SEPTEMBER 30

THURSDAY MORNING

8:00

- BREAKFAST -

SESSION ThM1 - Chair, Thomas Orlando

9:00 **INVITED - Electron Resonances in DIET**

Léon Sanche, *Université de Sherbrooke*

9:40 **Molecule Adsorbed on Rare-Gas Layers: Electron to Molecule Energy Transfer Mediated by Negative Ion Resonances**

C. D. Marinica, D. Teillet-Billy, and J. P. Gauyacq, *Université Paris-Sud*

10:00 **Absolute Measurement of Total Photo Desorption Yield of Solid Ne in Vacuum Ultraviolet Range**

I. Arakawa (1,2) T. Adachi (1), and T. Hirayama (1), (1) *Department of Physics, Gakushuin University*, (2) *Institute for Molecular Science, Okazaki*

10:20

- COFFEE BREAK -

SESSION ThM2 - Chair, Bruce E. Koel

10:50 **Effects of Morphology in Electron-Stimulated Desorption**

R. Azria, Y. Le Coat (1), M. Lachgar (1), Michel Tronc (2), L. Parenteau (3), and L. Sanche (3); (1)*Université Paris-Sud*, (2) *Université Pierre et Marie Curie*, (3) *University of Sherbrooke*

11:10 **Giant Cl⁻ and F⁻ Enhancements in Electron-Stimulated Desorption of CF₂Cl₂ Coadsorbed with Water or Ammonia Ices: Implications for Atmospheric Ozone Depletion**

Q.-B. Lu and Theodore E. Madey, *Rutgers, The State University of New Jersey*

11:30 **DIET and Reactive Scattering of Low Energy Cations (< 5 eV) in Molecular Surface Ices: Synthesis of New Chemical Species and Small Hydrocarbon Chains Initiated by Low Energy Electron Impact**

M. A. Huels, L. Parenteau, and L. Sanche, *University of Sherbrooke*

12:00

- LUNCH -

THURSDAY AFTERNOON

SESSION ThA1 - Chair, E. Malcolm Williams

- 1:20 **INVITED - Ion Desorption Induced by Core-Electron Transitions Studied with Electron-Ion Coincidence Spectroscopy**
K. Mase, *Institute for Molecular Science, Okazaki*
- 2:00 **Photo-Stimulated Ion Desorption from TiO₂ (110) Surface**
S. Tanaka, K. Mase, M. Nagasono, and M. Kamada, *Institute for Molecular Science, Okazaki*
- 2:20 **Energy Space Density Space Dynamics of DIET and DIMET Processes**
H. Guo, *University of New Mexico*
- 2:40 **DIET of Biological Molecular Systems Chemisorbed onto a Surface**
H. Abdoul-Carime, P. C. Dugal, and L. Sanche, *Université de Sherbrooke*
- 3:00 - COFFEE BREAK -

SESSION ThA2 - Chair, Katsumi Tanimura

- 3:30 **AFM and Time-Of-Flight Studies of Electron-Stimulated Desorption Processes in Bulk Single Crystals and Thin Epitaxial Layers of Alkali Halides**
M. Szymonski, B. Such, P. Struski, J. Kolodziej, P. Czuba, and P. Piatkowski, *Jagiellonian University*
- 3:50 **New Insight into Potential Sputtering of Insulators**
G. Hayderer, C. Lemell, L. Wirtz, M. Schmid, J. Burgdörfer, P. Varga, H. P. Winter and F. Aumayr, *TU Wien (Vienna University of Technology)*
- 4:10 **Observation of Surface Modification Induced by Bombardment of Highly Charged Ions**
R. Minniti, L. P. Ratliff, and J. D. Gillaspay, *NIST*
- 4:30 **Electron Stimulated Desorption of Hydrogen and Deuterium from Silicon (111) Surfaces Detected by Second Harmonic Generation**
M. Albert, G. Luepke, N. Tolk, *Vanderbilt University*
- 4:50 **Laser Induced Desorption from Metals**
D. P. Taylor and H. Helvajian, *The Aerospace Corporation*
- 5:10 **Desorption and Ablation of Diamond by Ultra-Short Laser Radiation**
V. Schmidt (1), W. Husinsky (1), Z. Marka (2), G. Betz (1), and N. Tolk (1, 2);
(1) *Vienna University of Technology*, (2) *Vanderbilt University*
- 6:00 - DINNER -
- 7:30 - 9:30 - POSTER SESSION -

FRIDAY OCTOBER 1

FRIDAY MORNING

8:00 - BREAKFAST -

SESSION FrM1 - Chair, Marek Szymonski

9:00 INVITED - Desorption Induced by Electronic Transitions of Alkali Metal Atoms and Oligomers from the Surface of Superfluid Liquid Helium Droplets

G. Scoles, *Princeton University*

9:40 DIET of Metastable Kr* Atoms via Electron Resonances in Kr/Ar Alloy Films

A. D. Bass, E. Vichnevetski and L. Sanche, *Université de Sherbrooke*

10:00 Electron-Stimulated Desorption of K and I from KI(100): Yields, Threshold Energies, and Velocity Distributions

A. Alexandrov(1), M. T. Sieger(1), R. G. Tonkyn(1), T. M. Orlando, N. Zema(2), and M. Piacentini(3); (1) *Pacific Northwest National Laboratory*, (2) *CNR*, (3) *Universita di Roma*

10:20 - COFFEE BREAK -

SESSION FrM2 - Chair, Robert A. Bartynski

10:50 INVITED - Surface Transition State Spectroscopy: Femtosecond Dynamics of Photodesorption of Cs from Copper

H. Petek, *Hitachi, Japan*

11:10 Laser-Induced Electronic Bond Breaking and Desorption of Constituent Atoms on InP(110)-(1x1)

Jun'ichi Kanasaki, Noriaki Mikasa, Shinsuke Kotake, and Katsumi Tanimura, *Nagoya University*

11:30 Time-Resolved Femtosecond Laser Induced Desorption from Magnesium Oxide and Lithium Fluoride Single Crystals

Alan G. Joly, Kenneth M. Beck, and Wayne P. Hess, *Pacific Northwest National Laboratory*

12:00 - LUNCH -

1:00 DEPARTURE

Poster Presentations

** Competing for Student Award

1. **Electron-Stimulated Desorption of Lithium Atoms from Oxidized Molybdenum Surfaces**
V. N. Ageev (1), Yu. A. Kuznetsov (1), and T. E. Madey (2); (1) *A. F. Ioffe Institute, St. Petersburg, Russia*, (2) *Rutgers University*
2. **Electron-Stimulated Desorption of Lithium Ions from Silicided Tantalum Surfaces,**
V. N. Ageev and S. M. Solovev, *A. F. Ioffe Institute, St. Petersburg, Russia*
3. **ESD and PSD of Alkalies from Oxide Surfaces - Relevance to Tenuous Planetary Atmospheres**
B. V. Yakshinskiy and Theodore E. Madey, *Rutgers University*
4. **Low-Temperature Water Ice Phases Probed by Electron Stimulated Desorption**
T. M. Orlando, M. T. Sieger and W. R. Wiley, *Pacific Northwest National Laboratory*
5. **Electron-Induced Processes in Condensed Films of CF_2Cl_2**
M. N. Hedhili (1), Q. B. Lu (1), T. E. Madey (1), M. Lachgar (2), Y. Le Coat (2), R. Azria (2), and M. Tronc(3); (1) *Rutgers University*, (2) *Université Pierre et Marie Curie*, (3) *Université Paris-Sud*
6. **Photon Stimulated Ion Desorption of Poly-Methylmethacrylate and Poly-Isopropenylacetate Thin Films following Oxygen Core Excitation**
K. Fujii**, S. Wada, D. Taga, Y. Nakashima, T. Sekitani and K. Tanaka, *Hiroshima University*; M. Tooyama, *Mitsubishi Rayon Co., Ltd., Otake, Japan*
7. **A Study of Photon Induced Processes with Adsorption-Desorption of Glycine at the $\text{TiO}_2(110) (1 \times 2)$ Surface**
E. Soria (1), I. Inmaculada (2), E. Roman (3), E.M. Williams (4), and J.L. de Segovia (1); (1) *CETEF "L. Torres Quevedo"*, (2) *Universidad Carlos III*, (3) *CSIC*, (4) *The University of Liverpool*
8. **Time-Of-Flight Techniques for the Investigation of Kinetic Energy Distributions of Ions and Neutrals Desorbed by Core Excitations**
R. Weimar (1), R. Romberg (1), S. Frigo (2), B. Kassuehlke (1), and P. Feulner (1); (1) *Technische Universität München*, (2) *Advanced Photon Source, Argonne*
9. **PSD of Neutral Hydrogen Atoms from Condensed Water and Ammonia by Resonant O1s and N1s Excitation: Search for the Signature of Ultrafast Bond Breaking**
R. Romberg**, S. Frigo (1), A. Ogurtsov (2), P. Feulner, and D. Menzel, *Technische Universität München*; (1) *Advanced Photon Source*, (2) *Verkin Institute for Low Temperature Physics & Engineering, Kharkov, Ukraine*

10. **A New Analyser for Gas and Ion Analysis: The Splat Analyser**
Robert G. Jones and N.E. Abrams, *University of Nottingham*
11. **Photon and Electron Stimulated Desorption of Excimers from the Surface of Solid Neon**
T. Adachi(1), T. Hirayama(1), and I. Arakawa(1, 2); (1) *Gakushuin University*
(2) *Institute for Molecular Science, Okazaki*
12. **H⁺ Desorption and Hydrogen Pairing on the Hydrogenated Si(100) Surface**
S. Vijayalakshmia, H. T. Liub and Z. Wu, *Rutgers University- Newark*
13. **Electron Stimulated Desorption and Fragmentation of Physisorbed Ferrocene Studied by STM**
K. Svensson, T. R. Bedson and R. E. Palmer, *The University of Birmingham*
14. **New Close-Coupling Approach for Ion-Surface Interactions, Including Continuum Discretization**
B. Bahrim and U. Thumm, *Kansas State University*
15. **Electron Stimulated Dissociation of Ammonia on Ge(100)**
C. Bate, M. Sanders, J. H. Craig, Jr., *University of Texas*
16. **Electron-Beam Induced Damage of Molecular Solids Containing Polyatomic Anions**
N. G. Petrik, G. Teeter, M. T. Sieger and T. M. Orlando, *Pacific Northwest National Laboratory*
17. **"DIET" in the bulk: X-ray excitation of DX centers in AlGaAs**
Yeong-Ah Soh and G. Aeppli *NEC Research Institute, E. D. Isaacs Lucent Technologies*, Frank M. Zimmermann, *Rutgers University*
18. **"Dissociative Adsorption and Recombinative Desorption of H₂ on Si(100): Solution of the "barrier puzzle""**, Frank M. Zimmermann and X. Pan, *Rutgers University*
19. **The Interaction of Low-Energy Molecular Ions with Surfaces**
Z. Marka, Y. Yao, B. Pratt-Ferguson, M. M. Albert, R. G. Albridge, G. L. Lüpke, A. Puckett, and N. H. Tolk, *Vanderbilt University*, G. Betz and W. Husinsky, *Technical University, Austria*, J. C. Tully, *Yale University*

TUESDAY SEPTEMBER 28

TUESDAY MORNING

8:00 - BREAKFAST -

SESSION TuM1 - Chair, Frank M. Zimmermann

8:50 Opening Remarks, T. E. Madey, *Rutgers University*

9:00 INVITED - DIET-Related Processes in Atomic Manipulation
G. Dujardin, *Université Paris-Sud, Orsay*

9:40 Vibrational Excitation and Electron Induced Dissociation by the STM: Pyridine and Benzene on Cu(001)
L. J. Lauhon** and W. Ho, *Cornell University*

10:00 Dynamics of Photodissociation of Adsorbed Nitrites on Ag(111): Rotationally Resolved Resonance Enhanced Multiphoton Ionization Time-of-Flight (REMPI-TOF) NO Spectra
Wei Zhao**, Chulhoon Kim, and J. Mike White, *The University of Texas at Austin*

10:20 - COFFEE BREAK -

SESSION TuM2 - Chair, Roger Azria

10:50 INVITED - Recent Progress in the Investigation of Core Hole-Induced PSD From Adsorbates: Excitation Site Dependent Bond Breaking, and Charge Rearrangement
P. Feulner, *Technische Universität München*

11:30 Photodesorption of Molecular Nitrogen from Pt(111)
C. French, B.C. Haynie, A. Solodukhin, I. Harrison, and R. Zehr**, *University of Virginia*

12:00 - LUNCH -

** Competing for Student Award

Tu-9:00 INVITED - "DIET-Related Processes in Atomic Manipulation"

G. Dujardin, *Université Paris-Sud, Orsay.*

Experiments on individual atoms and molecules using the Scanning Tunneling Microscope (STM) have opened up fascinating new areas of research. It has now become possible to fabricate atomic-scale structures of any desired geometry and to study their unique physical, chemical or electronic properties. By using the tip of the STM as an atomic-size electron source, a large variety of elementary manipulations can be performed; fragmentation of individual surface chemical bonds. However, the control and the understanding of these DIET-related processes engage fundamental new ideas and new concepts on inelastic electron effects on surfaces. Indeed, the specific physical processes occurring under the tip of the STM involve (i) the atomic-scale confinement of inelastic electron interactions, (ii) the injection of electrons below the vacuum level through the tunnel barrier, (iii) extremely high electron current densities. The precise understanding of these effects, which is still under debate, appears to be a big challenge for the development of atomic-scale technologies.

Tu-9:40 "Vibrational Excitation and Electron Induced Dissociation by the STM: Pyridine and Benzene on Cu(001)", L. J. Lauhon and W. Ho, *Cornell University*.**

The scanning tunneling microscope (STM) is a useful tool for the observation and chemical manipulation of molecules adsorbed on solid surfaces. The imaging capabilities of the STM are well known. In addition, tunneling electrons with energies of a few eV are capable of initiating chemical transformations confined to selected molecules. By performing inelastic electron tunneling spectroscopy with the STM (STM-IETS), the diagnostic capabilities of the STM are extended to include chemical sensitivity. The combination of these capabilities in a variable temperature STM allows DIET-like processes to be studied on the atomic scale for a wide range of systems.

We have studied benzene and pyridine adsorbed on Cu(001) at ~8 K. The bonding geometry of pyridine is very different from benzene due to the substitution of one nitrogen atom for a benzene C-H group. The difference is manifest in two experimental results. First, a C-H stretch mode is seen for pyridine but not benzene in STM-IETS. Second, the tunneling electron induced dissociation of these molecules shows a strong isotope effect for benzene but not pyridine. These two observations are connected by an understanding of how bonding affects the electronic and vibrational excitation and deexcitation of molecules. The reaction products of the STM induced dissociation were analyzed by imaging and STM-IETS. The bonding geometry changes upon dissociation and as a result, a C-H stretch mode is observed for both reaction products. These results, combined with previous studies of the thermal dissociation of pyridine, suggest the identities of the products, thus making a connection with dissociation induced by thermal excitations. Interestingly, the reaction pathway followed in STM induced dissociation is very different from that seen in photon induced dissociation of benzene and pyridine in the gas phase.

Preliminary experiments on the STM induced dissociation of acetylene (C_2H_2) and its isotopes (C_2HD , C_2D_2) show a difference in product yield (CCH, CC) between dissociation induced by highly localized tunneling electrons (0-4 eV) and more widely distributed field emitted electrons (4-10 eV). Complementary information is provided by the spatial mapping of the vibrational intensity of the acetylene C-H stretch. The mechanism responsible for the STM-IETS signal depends on coupling between energetic tunneling electrons and vibrational excitations of the adsorbate. Because an understanding of DIET processes proceeds with the elucidation of the microscopic mechanisms of such energy transfer, STM-IETS and STM induced dissociation are appropriately considered as DIET processes in a broad sense.

** Competing for Student Award

Tu-10:00 "Dynamics of Photodissociation of Adsorbed Nitrites on Ag(111): Rotationally Resolved Resonance Enhanced Multiphoton Ionization Time-of-Flight (REMPI-TOF) NO Spectra", Wei Zhao**, Chulhoon Kim, and J. Mike White, *The University of Texas at Austin*.

The dynamics of nitric oxide, NO, produced by 248 nm photodissociation of t-butyl nitrite, $(\text{CH}_3)_3\text{CONO}$, adsorbed on Ag(111) from submonolayer to multilayer regime has been studied using the resonance enhanced multiphoton ionization time-of-flight (REMPI-TOF) technique. REMPI-TOF spectra of NO ejected from the surface are sensitive to the rotational states of NO and the surface coverage and the structure of t-butyl nitrite. A REMPI-TOF spectrum of NO at high rotational states ($J > \sim 40.5$) shows a sharp peak of fast collisionless ejection along with an intermediate peak due to collisional energy loss of nascent NO to neighboring molecules. The collisionless peak is an evidence of direct excitation of t-butyl. As J is lowered, the intermediate peak position changes from 60 % of the collisionless kinetic energy down to 25%. A low J ($< \sim 20.5$) spectrum shows a low peak thermalized to the surface temperature. The relative intensity changes of collisionless, collisional and thermalized peaks as a function of surface coverage have been measured up to 40 ML t-butyl nitrite on Ag(111). The experimental results support the collisional model of NO ejection previously proposed by Fieberg and White. Angle dependent REMPI-TOF spectra of ejection NO gives some information on the alignment of t-butyl nitrite on the surface.

** Competing for Student Award

Tu-10:50 INVITED - "Recent Progress in the Investigation of Core Hole-Induced PSD From Adsorbates: Excitation Site Dependent Bond Breaking, and Charge Rearrangement", P. Feulner, R. Romberg, S. Frigo(1), R. Weimar, A. Ogurtsov(2), and D. Menzel, *Technische Universität München*, (1) *Advanced Photon Source, Argonne*, (2) *Verkin Institute for Low Temperature Physics & Engineering*.

Photodesorption and photofragmentation of adsorbed molecules by core electron excitation has attracted constant interest throughout the existence of this conference series. Reasons are i) that by their electronic decay primary core excitations serve as a source for strongly antibonding and well localized valence states which cause bond breaking even if lateral and vertical electronic quenching is fast, as for chemisorbates on metal surfaces; ii) that the distinct lifetime of core holes is an ideal internal clock which permits studies of the dynamics of the photochemical processes; and iii) that the allocation of the excitation to a distinct atom allows us to start the reaction at a definite site, at least for heteronuclear molecules. A comprehensive investigation of core level induced PSD from chemisorbates on metals is hampered by the fact that due to the very effective substrate-adsorbate charge transfer most of the molecules and fragments desorb neutrally, at least in the near threshold region, and are difficult to detect. Since our first PSD study of neutral fragments (S. Frigo et al., PRL **80**, 2813) the analytical tools for neutrals have been considerably improved, giving access not only to the spectral shape of the PSD yield, even under high resolution conditions and for "difficult" species as hydrogen atoms, but also to the kinetic energy distributions of desorbing particles (see also the contributions by R. Romberg et al. and R. Weimar et al. in this volume). A perspective overview is given on the importance of neutral PSD by core excitation and charge transfer reactions, using selected examples of PSD from CO and N₂ adsorbed in well ordered monolayers on metal surfaces. Special emphasis is laid on perpendicularly chemisorbed N₂ on a Ru surface. Chemisorption removes the symmetry of the molecule, shifts the excitation and ionization energies of the two atoms by different amounts compared with the isolated particle, and enables selective π -resonant N1s excitation either of the atom directed towards the substrate, or of that at the vacuum interface. It is shown that the branching into different PSD channels (neutral molecules, neutral fragments, and a tiny amount of N⁺) depends strongly on the excitation site. These findings are discussed using literature data on electronic decay under identical excitation conditions. We finally focus on N⁺ and N²⁺ PSD from chemisorbed N₂ stimulated by core hole excitation in the substrate. Under high resolution conditions distinct shifts of the threshold energy appear between photoabsorption and PSD which conclusively indicate direct coupling. Possible mechanisms are discussed.

Supported by the Deutsche Forschungsgemeinschaft (SFB 338 C10, Me 266/21-1; 2).

Tu-11:30 "Photodesorption of Molecular Nitrogen from Pt(111)", C. French, B.C. Haynie, A. Solodukhin, I. Harrison, and R. Zehr, *University of Virginia*.

Photochemistry of weakly adsorbed molecules on metal surfaces is often driven by photoexcited substrate electrons. We studied the photoinduced electron harpooning of physisorbed nitrogen on a Pt(111) surface at low temperature by monitoring the dynamics and photodesorption yield of nitrogen. The nitrogen adsorbate was initially characterized by thermal programmed desorption (TPD), reflection-absorption infrared spectroscopy (RAIRS), and by x-ray photoelectron spectroscopy (XPS). The photodesorption dynamics were studied by laser induced time of flight mass spectroscopy.

TPD showed a broad defect band at 65-110K at low exposures. A sharp peak appeared at 52K and decreased to 45K at higher exposures. The desorption of nitrogen at the 52K peak was best fit by first order kinetics until 0.15 monolayer exposure, whereupon it switched to zeroth order behavior. Nitrogen adsorbed onto Pt(111) shows a two phase behavior similar to that reported of rare gasses adsorbed onto close packed metal surfaces. In the rare gas systems the adsorbate forms a dilute 2D gas at low coverage. As the coverage increases, a condensed island phase forms which coexists with the 2D gas phase. RAIRS showed an absorbance at 2266cm^{-1} for terrace nitrogen and 2234cm^{-1} for nitrogen adsorbed at the step edge defects. The assignment of the 2234cm^{-1} band was done based on a CO titration of the step edges which removed the 2234cm^{-1} signal. The RAIRS data supported the two phase model. The integrated absorbance of terrace nitrogen at 2266cm^{-1} remained zero until an exposure of 0.17 ML, afterwards it increased linearly with exposure until it saturated around 0.6 ML exposure. The XPS results gave a (1s) peak at a binding energy of 403.5-403.8 eV with a fwhm of 1.5 eV. This was assigned to physisorbed nitrogen by comparison to the physisorbed peak of nitrogen on graphite which has an $E_b(1s)=403.9\text{ eV}$.

Nitrogen was found to desorb upon illumination by ultraviolet laser at wavelengths of 193 nm, 266 nm, and 308 nm. No detectable photodesorption was found for illumination at 532 nm. The mean translational energy of desorbing nitrogen was found to be 0.2 eV with the maximum being approximately 0.8 eV. The TOF spectra were bimodal, having a fast and a slow peak. The fast peak had a mean translational energy of 0.48 eV, compared to the slow peak's value of 0.08 eV. The fast peak was attributed to nitrogen photodesorbed directly from the surface. The slow peak was thought to be due to photodesorbed nitrogen undergoing inelastic collisions in the adlayer. The photoactivity was shown to be due to defect sites by annealing to 60K to desorb the terrace nitrogen and irradiating. The photodesorption yield was found to increase by 40% compared to dosing and irradiation at 27K. The photochemical cross sections were measured as a function of exposure for 193nm and 266nm. Both cross sections showed a maximum value at low exposure that rapidly decreased to a steady value at exposures greater than 0.17 monolayer. These results indicate that the 2D gas phase is photoactive. Photodesorption yield by TOF also corroborates this model. The photodesorption yields at 193nm at a constant photon flux increases monotonically with increasing exposure until an exposure on 0.17 monolayers whereupon the yield remains constant. TOF polarization experiments were also conducted. The photodesorption yields for the ratio of *p* versus *s* polarized 193nm light tracked the calculated ratio of the absorbences of *p* versus *s* polarized light by the platinum substrate. The yield variation, along with the fact that the mean translational energy for 193nm and 308nm were the same are indicative of a mechanism that involves transient attachment of photogenerated hot carriers.

****Competing for Student Award**

TUESDAY SEPTEMBER 28

AFTERNOON

SESSION TuA1 - Chair, Dietrich Menzel

- 1:20 **INVITED - Stimulated Desorption by Electron Standing Waves**
M. T. Sieger, *Pacific Northwest National Laboratory*
- 2:00 **Discriminating Time and Angles: TOF-ESDIAD Studies of Interactions between Particles Adsorbed on a Single Crystal Metal Surface**
Dan Mocuta^{**}, Joachim Ahner, and John T. Yates, Jr., *University of Pittsburgh*
- 2:20 **Electron Beam Induced Degradation of Zinc Sulfide-Based Phosphors**
B. L. Abrams^{**}, W. Roos, and P. H. Holloway, *University of Florida*
H. C. Swart, *University of the Orange Free State*
- 2:40 **Electronic Sputtering of Condensed Gas Solids**
E. M. Bringa^{**} and R. E. Johnson, *University of Virginia*
- 3:00 - COFFEE BREAK -

SESSION TuA2 - Chair, David Langreth

- 3:30 **INVITED - Molecular Desorption from Surfaces - A Testing Ground for Dissipative Quantum Dynamics**
Shiwu Gao, *Chalmers University*
- 4:10 **A First Principles Study of Laser Induced Desorption: Ab Initio and Wave Packet Calculations**
T. Klüner, S. Thiel, and H.-J. Freund, *Fritz-Haber-Institut, Berlin*
V. Staemmler, *Ruhr-Universität Bochum*
- 4:30 **Dissociation of an Adsorbate Surface Bond by Direct Optical Excitation: H-Si(100)**
T. Vondrak and X.-Y. Zhu, *University of Minnesota*
- 4:50 **Photodesorption and Electronic Relaxation**
G. Comtet, L. Hellner, G. Dujardin, and V. Bellanger, *Universitaire Paris-Sud*
- 5:10 **Photodissociation of CH₃I/Cu(110): Surface Effects in Dissociation Pathways**
C.C. Johnson and E.T. Jensen, *University of Northern British Columbia*
- 6:00 - DINNER -
- 7:30 - 9:30 - POSTER SESSION -

^{**}Competing for Student Award

Tu-1:20 INVITED - "Stimulated Desorption by Electron Standing Waves", M. T. Sieger, G. K. Schenter, and T. M. Orlando, *Pacific Northwest National Laboratory*

An issue central to understanding DIET is the relationship between the atomic and electronic structure of a surface species and its desorption probability. Given a flux of desorption products entering a detector, one would like to know where the particles were produced in the solid and the excitation process responsible for their emission. Current models of ESD describe the total desorption cross section as the product of the excitation (inelastic electron-solid scattering) cross-section and the desorption or escape probability. The vast majority of effort in experimental and theoretical ESD has focused on the dynamics of the desorption process, and on final-state kinetic energy and/or desorption trajectory distributions, with the assumption that the inelastic electron-solid scattering cross-section is a fixed function of electron energy.

However, there are also initial-state effects in ESD which can affect the excitation cross section. We report calculations and experiments demonstrating that total ESD yields show fine-structure with incident electron direction, consistent with quantum-mechanical scattering and interference in the initial state of the desorption process. In a time-independent picture, interference of the incident plane wave with waves scattered from the crystalline lattice forms an electron standing wave (ESW), having spatially localized maxima and minima in the incident electron density. Whether a particular point on a surface experiences a maximum or minimum depends on the wavelength of the electron, the direction of incidence relative to the crystal axes, and the locations of nearest neighbor atoms. Since the probability of excitation is proportional to the incident electron density at or near the site of the "absorber" atom (the site of the inelastic scattering event), the total ESD rate should depend upon the local atomic structure and the k -vector of the incident wave. The total desorption yield, when measured as a function of incident direction at constant energy, shows oscillations with the symmetry of the absorber bonding site. These oscillations are represented as a χ -function, characterizing the deviation in the yield due to diffraction, where the total yield is $I(k) = I_0 (\chi(k) + 1)$. Every inequivalent atomic bonding site has a unique χ -function, so measurements of $I(k)$ can in principle uniquely determine the bonding geometry of the absorber.

Electron standing wave stimulated desorption (ESWSD) can provide detailed information about the ground state surface bonding geometry of the absorber with sub-angstrom resolution of bond vectors. We discuss the role of electron diffraction in ESD, and present experimental measurements for chlorinated Si surfaces.

Tu-2:00 "Discriminating Time and Angles: TOF-ESDIAD Studies of Interactions Between Particles Adsorbed on a Single Crystal Metal Surface", Dan Mocuta, Joachim Ahner and John T. Yates, Jr., *University of Pittsburgh***

Since its discovery in 1974 [1] electron stimulated desorption ion angular distribution *ESDIAD* has been used to extract information about the orientation and dynamics of molecules adsorbed at metallic, semiconductor or insulator single crystal surfaces. A recent development [2] of the digital *ESDIAD* technique permits simultaneous monitoring of each electron stimulated desorption event by measuring each particle's time of flight as well as desorption angle. The comprehensive analysis of the time-angular data set allows the inference of structural and dynamical [3] information on the interadsorbate as well as adsorbate-substrate interactions which in some cases are not accessible to other techniques, as will be shown.

The well defined angular distributions obtained by the O^+ ions desorption from the striped $O(2\times 1)$ -Cu(110) caused by electronic excitation have been used to study the thermally activated growth and coverage dependency of the stripes. It has been found that O atoms from the central regions of the stripes may be distinguished from O atoms at the stripe edges and that the cross section for O^+ production increases when a chemisorbed O atom is converted to a component of the stripes. Thermal broadening effects in the one dimensional O-Cu-O-Cu chains forming the oxide stripes has been studied.

Time of flight separation of ions and excited neutrals with different masses permitted the simultaneous detection of the *ESDIAD* patterns of O^+ , CO^+ and CO^* from CO coadsorbed on the striped $O(2\times 1)$ -Cu(110) structure. A strong interaction of the CO molecules with oxygen atoms situated at the stripe edges was inferred from the decrease of the O^+ ion signal originating from these sites. At 67 K CO molecules physisorbed on the oxide stripes have been imaged. A similar experiment involving Ar atoms has been performed on the striped oxidized Cu(110) surface at 32 K. The Ar atoms are trapped only at the oxide stripe edges at this temperature and strongly quench O^+ emission from the stripe edges. The similarities and differences with the CO/O-Cu(110) system are analyzed.

[1] J. J. Czyzewski, T. E. Madey, and J. T. Yates, Jr., *Phys. Rev. Lett.* **32**, 777 (1974)

[2] J. Ahner, D. Mocuta, and J. T. Yates, Jr., *Jour. Vac. Sci. Technol. A*, Jul/Aug 1999.

[3] J. Ahner, D. Mocuta, and J. T. Yates, Jr., *Phys. Rev. Lett.* **79**, 1889 (1997).

****Competing for Student Award**

Tu-2:20 "Electron Beam Induced Degradation of Zinc Sulfide-Based Phosphors", B.L. Abrams**, W. Roos, P.H. Holloway, *University of Florida*, H.C. Swart, *University of the Orange Free State*

The change in cathodoluminescent (CL) brightness and changes in the surface chemistry of SiO₂-coated and uncoated ZnS:Ag, Cl powder phosphor have been investigated using a scanning Auger electron spectrometer and an Oriel optical spectrometer. The data were collected in a stainless steel UHV chamber with residual gas pressures of 1x10⁻⁸ Torr and 1x10⁻⁶ Torr. The primary electron current density was varied from 100 to 1000 μA/cm² but was normally 270 μA/cm². The primary electron beam energy was varied between 2keV and 5keV. In the presence of a 2keV primary electron beam in 1x10⁻⁶ Torr of water, the amounts of C and S on the surface decreased while the O concentration increased. XPS data showed that ZnO formed on both the coated and uncoated samples. This change in surface chemistry coincided with a decrease in CL brightness. Our model of electron beam stimulated surface chemical reactions (ESSCR) for this degradation process postulates that the primary and secondary electrons dissociate physisorbed molecules to reactive atomic species. These atomic species remove surface S and C as volatile SO_x and H₂S species allowing formation of a non-luminescent ZnO layer in 1x10⁻⁶ Torr water. However, in a vacuum of 1x10⁻⁸ Torr dominated by hydrogen and with a low water content, there was no decline in S, no rise in O, but the CL still degraded. These effects are still attributed to ESSCR with hydrogen assisted by thermal effects. Hydrogen is postulated to dissociate under the electron beam and remove S as H₂S while Zn volatilizes due to a high vapor pressure and elevated temperatures from electron beam heating. SEM images of the SiO₂-coated samples after degradation at 2keV revealed etching and pitting of the surface especially near SiO₂ particulates. Surface deterioration was very dramatic for a 5keV primary electron beam. Only a small decrease in CL brightness and no morphology change was detected for uncoated samples. This suggests that SiO₂ acted as a catalyst for decomposition.

This work was supported by DARPA Grant MDA 972-93-1-0030 through the Phosphor Technology Center of Excellence.

****Competing for Student Award**

Tu-2:40 " Electronic Sputtering of Condensed Gas Solids", E. M. Bringa and R. E. Johnson, *University of Virginia***

The bombardment of low temperature condensed gas solids by MeV light ions produces electronic excitations that can decay non-radiatively. These events transfer kinetic energy to the lattice causing ejection (sputtering) of atoms near the surface. The electronic sputtering of these materials is of interest as it produces atmospheres on the moons of Jupiter and gives insights to the non-radiative decay processes. The experimental data for the electronic sputtering yield, Y , of solid O_2 and N_2 , shows two regimes as a function of the energy deposited per unit path length, dE/dx . At low dE/dx , $Y \sim dE/dx$, while at high dE/dx , $Y \sim (dE/dx)^2$ [1]. Parametrizing an analytical thermal spike model with constant track radius gave very satisfactory agreement with the data [2]. However, molecular dynamics (MD) calculations have shown that the thermal spike model does NOT give a satisfactory description of sputtering and energy transport for solid O_2 [3]. MD gives $Y \sim dE/dx$ at HIGH dE/dx for constant track radius, despite the non-linearity of the sputtering process. The quadratic dependence in the experimental data could be due to two reasons. First, the size of the initially excited track may be INCREASING with dE/dx [4], contrary to the dependence predicted by the Bohr adiabatic radius. This may be due to exciton diffusion prior to decay. Second, the energy deposited in the lattice may be non-linear in dE/dx [5], as in the Coulomb explosion mechanism. Since the solids of interest, O_2 and N_2 , have internal degrees of freedom, the role of the vibrational energy transport from the excited track will also be examined.

[1] K. Gibbs, W. L. Brown, and R. E. Johnson, Phys. Rev. B **38**, (1988) 11001. W. L. Brown, L. J. Lanzerotti, K. J. Marcantonio, R. E. Johnson and C. T. Reimann, Nucl. Instr. and Meth. B **14**, (1986) 392.

[2] R. E. Johnson, M. Pospieszalka, and W. L. Brown, Phys. Rev. B **44**, (1991) 14.

[3] E. M. Bringa, R. E. Johnson and L. Dutkiewicz, Nucl. Instr. and Meth. B **152**, (1999) 267.

[4] E. M. Bringa and R. E. Johnson, submitted.

[5] C. Watson and T. Tombrello, Rad. Eff. **89** (1985) 263.

**Competing for Student Award

Tu-3:30 *Invited* - "Molecular Desorption from Surfaces--A Testing Ground for Dissipative Quantum Dynamics", Shiwu Gao, Chalmers University

This paper discusses the role of dissipation in the dynamics of molecular desorption on a model system, $O_2/Pt(111)$, where recent experimental data have documented detailed information about its reaction dynamics. First, the failure of the Schroedinger dynamics in the description of DIET is shown. A general Lindblad approach for dissipative quantum dynamics will be introduced. This approach is applied to describe DIET of the same system. It is shown that it overcomes the difficulties encountered in the Schroedinger dynamics. In a multi-dimensional (2D) system, the anisotropic dissipation is shown to determine decisively the selectivity of bond-breaking, here, the branching ratio between desorption and dissociation. With reasonable parameters, it is possible to reproduce the branching ratio of DIET measured experimentally. The effect of dissipation on the dynamics of multiple electronic transitions (DIMET) will also be possibly elaborated.

Tu-4:10 "A First Principles Study of Laser Induced Desorption: ab initio and Wave Packet Calculations", T. Klüner, S. Thiel, H. -J. Freund, Fritz-Haber-Institut der Max-Planck-Gesellschaft; V. Staemmler, Ruhr-Universität Bochum

We present a detailed first principles study of quantum state resolved laser induced desorption of NO from NiO(100). By performing high quality ab initio cluster calculations on the configuration interaction level we have been able to construct potential energy surfaces (PES) for the electronic states involved in the desorption process. For the first time it has been possible to calculate a PES for an excited electronic state of a molecule adsorbed on an oxide surface. The state can be characterized as a charge transfer state, in which an electron is transferred from the surface to the adsorbed molecule resulting in an NO⁻-like species with a full negative charge on the adsorbate. The topology of the excited state PES is analyzed in detail identifying the Coulomb attraction between NO⁻ and the hole created in the surface to be the driving force for an Antoniewicz-like desorption scenario. The topology of the PES with respect to a variation of the polar angle turns out to be crucial for the understanding of the dynamics of nuclear motion and for the interpretation of the experimental results.

We performed multi-dimensional wave packet calculations on our ab initio PES in order to simulate the rotationally and vibrationally state resolved velocity distributions. In case of a resonance lifetime of 25 fs quantitative agreement with all experimental observables (shape and vibrational excitation) was obtained. The bimodality of the velocity distributions could be traced back to a bifurcation during the propagation of the wave packet on the excited state PES due to its non trivial topology. A complete microscopic understanding of the experimental results has been obtained on a quantum mechanical basis [1, 2].

[1] T. Klüner, H. -J. Freund, V. Staemmler, R. Kosloff, Phys. Rev. Lett. **80**, (1998), 5208.

[2] T. Klüner, S. Thiel, V. Staemmler, H. -J. Freund, Chem. Phys. Lett. **294** (1998), 413.

Tu-4:30 "Dissociation of an adsorbate surface bond by direct optical excitation: H-Si(100)", T. Vondrak and X.-Y. Zhu, *University of Minnesota*

Direct photodissociation of an adsorbate-surface bond is achieved for Si(100)-(2x1):H monohydride surface at 157 nm [1]. We determined using polarized light that the transition dipole moment for the optical excitation is oriented at 18 degrees from surface normal, as expected for the σ - σ^* transition within the H-Si bond. The dynamics of this process is characterized by a translational energy of $\langle E \rangle = 0.24 \pm 0.02$ eV for atomic H and an isotope effect in photodesorption yield of 10 ± 3 . We carried out time-dependent quantum mechanical simulation on ab initio potential energy surfaces. The simulation reveals that the experimental isotope effect corresponds to an excited state lifetime of 0.4 fs and a quantum yield for atomic hydrogen desorption of 2×10^{-5} . This study provides an extreme example for bond-selective photochemistry in large chemical systems. In addition to its significance in understanding ultrafast DIET processes, the direct photodesorption process demonstrated here may also find applications as resistless photolithography in semiconductor technology.

[1] T. Vondrak and X.-Y. Zhu, Phys. Rev. Lett., 82 (1999) 1967-1970.

Tu-4:50 "Photodesorption and Electronic Relaxation", G. Comtet (1), L. Hellner (1, 2), G. Dujardin(1, 2), V. Bellanger (1); (1) *Laboratoire pour l'Utilisation du Rayonnement Electromagnétique, B.t. 209D Centre Universitaire Paris-Sud*, (2) *Laboratoire de Photophysique Moléculaire B.t. 210 Université Paris-Sud*

The dynamics of the desorption induced by electron excitation may be approached through the measurement of the yield and of the kinetic energy distribution of the desorbing particles. Further information is obtained by comparing these quantities for two isotopic species.

In the case of O_2 adsorbed on the Si(111)7x7 surface, the yields and the kinetic energy distributions of O^+ photodesorbed ions following photon excitation of the 1s core level of the oxygen adsorbate and of the 2p core level of the silicon substrate have been measured. In both cases, the yield of the heaviest O^+ isotope is the smallest and the kinetic energy distribution of the heaviest O^+ isotope is shifted down by about 0.6 eV. This last observation indicates that one needs to go beyond the well-known MGR model (named after Menzel, Gomer and Redhead). More complicated schemes involving at least three electronic states have to be considered to explain these results.

Tu-5:10 "Photodissociation of CH₃I/Cu(110): Surface Effects in Dissociation Pathways", C.C. Johnson and E.T. Jensen, University of Northern B.C

The photodissociation dynamics of gas phase CH₃I in the A-band ($h\nu=3.5$ to 5.6eV) is fairly well understood [1]. The strongest contribution to the A-band absorption is a repulsive state correlating to the formation of CH₃ + I* (³P_{1/2}), however in detection a large fraction of the dissociating molecules decay to CH₃ + I (²P_{3/2}, ground state) due to a curve crossing during dissociation. The relative amounts of I and I* formation vary considerably across the A-band. When CH₃I is adsorbed on a surface, the photodissociation dynamics have been found to be perturbed due to charge transfer, quenching and solid state effects [2,3]. In studying the adsorption and photodissociation of CH₃I on Cu(110) in the long wavelength tail of the A-band ($h\nu=3.68\text{eV}$), we have found that the dissociation dynamics are strongly perturbed from those in the gas phase. The flux of desorbing CH₃ fragments is strongly peaked away from the surface normal, indicating an ordered but tilted layer of CH₃I molecules at the surface. The photoyield of CH₃ as a function of coverage is strongly enhanced in the region of 2 to 4ML of adsorbate. Most strikingly, the observed branching in the I/I* channels (as judged by TOF measurements on the CH₃ fragments) is very different from expectations based on the gas phase, and found to favour the higher energy I* dissociation channel. This behaviour is the reverse of that seen for the same molecule at shorter wavelengths in the A-band on other surfaces [2,3]. In the present case we find the branching ratio to be $\Phi^* = \text{I}^* / (\text{I} + \text{I}^*) \sim 0.66$.

[1] A.T.J.B. Eppink and D.H. Parker, J. Chem. Phys. 109, 4758 (1998).

[2] E.T. Jensen and J.C. Polanyi, J. Phys. Chem. 97, 2257 (1993).

[3] S.R. Coon, K.B. Myli and V.H. Grassian, J. Phys. Chem. 99, 16416 (1995).

WEDNESDAY SEPTEMBER 29

MORNING

SESSION WeM1 - Chair, Norman Tolk

- 9:00 **INVITED - Adsorbate Photochemistry and Electron Chemistry**
John C. Polanyi, *University of Toronto*
- 9:40 **Photoexcited Electrons and Induced Vibrational Pre-Desorption on a Metal Surface**
Pui-Teng Howe and Hai-Lung Dai, *University of Pennsylvania*
- 10:00 **Energy-Resolved Angular Distributions for Photoinduced DEA to Methyl Bromide on GaAs(100): Photochemically-Induced Surface Reconstruction and Evidence for Site Specificity**
K. A. Khan, N. Camillone III, J. Yarmoff, and R. M. Osgood, Jr., *Columbia University*
- 10:20 - COFFEE BREAK -

SESSION WeM2 - Chair, Hai-Lung Dai

- 10:50 **Surface Dynamics Using Pulsed Electron Beams**
Ally S.Y. Chan and Robert G. Jones, *University of Nottingham*
- 11:10 **Selectivity of Bond-Breaking in Electron-Induced Dissociation (EID) of Hydrocarbon Films on Au Surfaces**
D. Semin and B. E. Koel, *University of Southern California*
- 11:30 **Photoinduced Hot Electron Transfer to Self-Assembled Monolayers of Molecular Quantum Dots on Metal Surfaces**
T. Vondrak and X.-Y. Zhu, *University of Minnesota*
- 12:00 - LUNCH -

**We-9:00 "Adsorbate Photochemistry and Electron Chemistry", John C. Polanyi,
University of Toronto**

Over the past years this laboratory has been exploring the photochemistry of a variety of molecules adsorbed in sub-monolayers or monolayers on single-crystal surfaces in ultrahigh vacuum. The adsorbate layer is in general ordered, due to adsorbate-substrate forces and adsorbate-adsorbate forces. Ordering has been shown by studies of the dynamics of photofragment recoil from the surface, as well as by polarised Fourier Transform Infrared (FTIR) spectroscopy. (1) We shall describe recent experiments¹ in which the dynamics of photo-recoil from the surface are modified by electron impact or H-atom impact on a $\text{CaF}_2(111)$ substrate, (2) Experiments² in which photo-recoiling Cl gives evidence of coming from the metastable species $\text{Cl}_2\cdot\text{Cl}$, (3) Experiments in which photofragments (e.g., atomic H recoiling from a sub-monolayer of HCl adsorbed on $\text{LiF}(001)$, photolysed at 193 nm), directed downward at an inert crystal surface recoil at non-specular angles indicative of 'Localized Atomic Scattering' (LAS)³. This is evidence that the scattered H, coming from ordered HCl(ad) , rebounds from selected atomic locations on the surface. In more recent work using a reactive rather than an inert substrate (namely $\text{Si}(111)$) it has been found by STM that the downward-directed photofragments or electron-impact-induced fragments (e.g., Cl atoms from chlorobenzene) react closely-adjacent to the 'parent' molecule (the chlorobenzene, in the example cited)⁴. This is clear evidence of 'Localised Atomic Reaction', (LAR). These and other systems involving the photodissociation and electron-impact dissociation of individual molecules, studied by Scanning Tunneling Microscopy (STM), will be described.

¹ T.G. Lee and J.C. Polanyi. To be published (1999).

² S.A. Raspopov, N.S.-K. Sze, F.Y. Naumkin, J.B. Giorgi and J.C. Polanyi; to be published (1999).

³ J.B. Giorgi, R. Kühnemuth and J.C. Polanyi, J. Chem. Phys. **110**, 598 (1999).

⁴P.-H. Lu, J.C. Polanyi and D. Rogers; to be published (1999).

We-9:40 "Photoexcited Electrons and Induced Vibrational Pre-desorption on a Metal Surface", Pui-Teng Howe and Hai-Lung Dai, *University of Pennsylvania*

When light is used to irradiate a system of small organic molecules (such as formaldehyde or ketene) weakly adsorbed on a metal surface (Ag) at low temperature (100K), it is observed that only a few molecules would have dissociation reaction induced by irradiation but nearly all display desorption. The desorption is observed even when photon energies are as low as 1.2 eV. The dissociation reactions, such as formaldehyde dissociation into methylene and oxygen, are induced by energetic electrons in the substrate excited by the photons. These hot electrons may tunnel to a dissociative negative ion state of the molecule and induce dissociation. Only molecules which have unstable negative ion states undergo dissociation.

The photoexcited electrons, including the ones excited by photons with energies as low as about 1 eV, can also cause the physisorbed molecules to desorb. Here, we propose a mechanism based on the following observations: all the desorbed molecules have low translational temperature, only molecules with an IR active vibrational modes with energy higher than the surface binding energy desorb, and the desorption probability is proportional to the transition dipole strength of the vibrational mode. In this mechanism, vibrational pre-desorption induced by photoexcited electrons in the substrate, the IR active modes of the molecular adsorbate are excited by hot electrons scattering off the surface. Energy transfer from the excited vibrational levels, with energy higher than the binding energy, to the substrate-adsorbate bond causes desorption.

We-10:00 "Energy-Resolved Angular Distributions for Photoinduced DEA to Methyl Bromide on GaAs(100): Photochemically-Induced Surface Reconstruction and Evidence for Site Specificity", K. A. Khan, N. Camillone III, J. Yarmoff and R. M. Osgood, Jr., *Columbia University*

Brominated hydrocarbons adsorbed on semiconductor surfaces serve as model systems for investigating the photoinduced electron chemistry of oriented molecules in the condensed phase. Using mass and angle-resolved time-of-flight (TOF) and temperature-programmed-desorption (TPD) measurements we have characterized the dynamics of the electron attachment process and subsequent fragmentation of methyl bromide (MeBr) adsorbed in monolayer and submonolayer quantities on the Ga c(8x2)- and As c(2x8)-terminated surfaces of GaAs(100). Pre-irradiation TPD measurements show that MeBr interacts more strongly with the As-terminated surface, and monolayer growth is nearly complete prior to the onset of multilayer growth. The interactions between MeBr and the Ga-terminated surface are weaker, resulting in a blurring of the distinction between monolayer and multilayer growth. The electron chemistry is initiated by irradiating the monolayers with low energy ($\sim 1 \text{ mJ/cm}^2$) excimer laser pulses at 193, 248 or 351 nm. Previous experiments on the (110) surface showed that MeBr dissociates via attachment of photoexcited substrate electrons resulting in cleavage of the C-Br bond. Following dissociation, the heavy bromine anion is trapped at the surface whereas the neutral alkyl radicals are ejected from the surface. For the (100) surfaces, angular distributions reveal a striking surface-structure dependence. For the Ga-terminated surface, no less than five distinct dynamical channels are observed: (1) ejection of $\sim 2 \text{ eV}$ methyl radicals into lobes peaked at $\sim \pm 60^\circ$ from the surface normal (along both the 8-fold and 2-fold azimuthal directions) (2) ejection of $\sim 1 \text{ eV}$ methyl radicals into lobes peaked at $\sim \pm 25^\circ$.

We - 10:50 "Surface Dynamics using Pulsed Electron Beams", Robert G. Jones and N.E. Abrams, *University of Nottingham*

We have used line of sight time of flight (LOSTOF) to measure the translational energy of ethene formed by dissociative electron attachment of adsorbed dihalocarbons on Cu(111) at 100 K. A pulsed electron beam (2 keV, 20 micro A, 500 micro s) was used to generate low energy secondary electrons at the surface, which were the active agents in the ensuing decomposition. $\text{dihalocarbon(ads)} + \text{low energy } e^- = \text{radical(ads)} + \text{halogen(chem)} + e^-$
 $\text{radical(ads)} = \text{ethene} + \text{halogen(chem)}$ For 1,2-dichloroethane (DCE) adsorbed with a spacer layer of chemisorbed chlorine between it and the Cu(111)surface, the TOF data could be fitted using three Maxwell distributions with temperatures of 1000, 200 and 20 K. The first two were due to surface reactions while the third, a spuriously low temperature, only occurred for multilayers and was due to diffusion of ethene through one or more layers of DCE. For a single monolayer of DCE adsorbed directly on the clean Cu(111) the hyperthermal component rose in energy to 1200 K, $E(\text{trans})=21.8 \text{ kJ / mol}$, indicating that the copper surface was affecting the reaction. For 1-bromo-2-chloroethane the results were the same, consistent with both molecules dissociating via a common intermediate, ClC_2H_4^* , $\text{ClC}_2\text{H}_4^* = \text{ethene} + \text{Cl(chem)}$. For 1,2-dibromoethane the intermediate must be different, BrC_2H_4^* , and indeed monolayer adsorption of this molecule on clean Cu(111) exhibited two Maxwell distribution with temperatures of 1800 K, $E(\text{trans})=29.9 \text{ kJ/mol}$ (much higher than) and 200K (about the same as) the other two molecules. The dynamics of these reactions and the origin of the two Maxwell distributions are discussed in terms of the energy available within the radical and from the formation of the chemisorbed halogen when the radical dissociates.

We-11:10 "Selectivity of Bond-Breaking in Electron-Induced Dissociation (EID) of Hydrocarbon Films on Au Surfaces", D. Semin and B. E. Koel, *University of Southern California*

Electron-induced dissociation (EID) processes in organic and polymer films are important in a variety of applications. One scientific issue concerns the selectivity of low-energy electron bombardment to cleave a single C-H bond in hydrocarbon condensed films or adsorbed layers. We have undertaken combined TPD and FT-IRAS studies to identify and determine the purity of the surface species produced by EID of several hydrocarbon films on Au(111), including cyclohexane, cyclohexene, and benzene layers. We also measured the EID threshold and cross sections for incident-electron energies in the range from zero to 50 eV. The thermal chemistry of the hydrocarbon films and the EID products was also investigated.

We-11:30 "Photoinduced Hot Electron Transfer to Self-Assembled Monolayers of Molecular Quantum Dots on Metal Surfaces", T. Vondrak and X.-Y. Zhu,
University of Minnesota

Aromatic molecules have recently been proposed and tested as quantum dots (QDs) in resonant and single electron transport structures. The key issue in designing these future devices is understanding the electronic interaction and the electron transfer mechanism between the organic molecule and the metal or semiconductor substrate. We demonstrate a successful approach to probe such an interfacial electronic structure and electron transfer using two-photon photoemission (2PPE) in a model system, self-assembled monolayer (SAM) of pentafluorothiophenolate, $\text{C}_6\text{F}_5\text{S}^-$, on Cu(111). We found that photo-induced hot electron transfer to the lowest unoccupied molecular orbital (LUMO) occurs at 3.2 eV below the vacuum level while coherent two photon ionization of the highest occupied molecular orbital (HOMO) occurs at 0.7 eV below the Fermi level. Compared to gas phase $\text{C}_6\text{F}_5\text{SH}$, the LUMO is stabilized by more than 3 eV in the SAM. This large stabilization energy is too large to be accounted for the charge-image potential and must involve strong electronic interaction, i.e., direct wavefunction mixing, between the molecular orbital and substrate electronic energy bands. Similar arguments apply to the $> 3\text{eV}$ stabilization of the photo-hole from the HOMO. These assessments are confirmed by electronic structural calculations. As expected, the strong electronic coupling in photoinduced electron transfer is absent when the molecule is not in direct contact with the surface, e.g., for C_6F_6 adsorbed in the second molecular layer on the Cu(111) surface.

THURSDAY SEPTEMBER 30

MORNING

SESSION ThM1 - Chair, Thomas Orlando

- 9:00 **INVITED - Electron Resonances in DIET**
Léon Sanche, *Université de Sherbrooke*
- 9:40 **Molecule Adsorbed on Rare-Gas Layers: Electron to Molecule Energy Transfer Mediated by Negative Ion Resonances**
C. D. Marinica, D. Teillet-Billy, and J. P. Gauyacq, *Université Paris-Sud*
- 10:00 **Absolute Measurement of Total Photo Desorption Yield of Solid Ne in Vacuum Ultraviolet Range**
I. Arakawa (1,2) T. Adachi (1), and T. Hirayama (1), (1) *Department of Physics, Gakushuin University*, (2) *Institute for Molecular Science, Okazaki*
- 10:20 - COFFEE BREAK -

SESSION ThM2 - Chair, Bruce E. Koel

- 10:50 **Effects of Morphology in Electron-Stimulated Desorption**
R. Azria, Y. Le Coat (1), M. Lachgar (1), Michel Tronc (2), L. Parenteau (3), and L. Sanche (3); (1)*Université Paris-Sud*, (2) *Université Pierre et Marie Curie*, (3) *University of Sherbrooke*
- 11:10 **Giant Cl⁻ and F⁻ Enhancements in Electron-Stimulated Desorption of CF₂Cl₂ Coadsorbed with Water or Ammonia Ices: Implications for Atmospheric Ozone Depletion**
Q.-B. Lu and Theodore E. Madey, *Rutgers, The State University of New Jersey*
- 11:30 **DIET and Reactive Scattering of Low Energy Cations (< 5 eV) in Molecular Surface Ices: Synthesis of New Chemical Species and Small Hydrocarbon Chains Initiated by Low Energy Electron Impact**
M. A. Huels, L. Parenteau, and L. Sanche, *University of Sherbrooke*
- 12:00 - LUNCH -

Th-9:00 INVITED - "Electron Resonances in DIET"

Léon Sanche, *Université de Sherbrooke*

Peaks or maxima, which appear in desorption yield functions, obtained by 5 to 20 eV electrons impinging from vacuum on atomic or molecular solid films, reveal the formation of transient anions (i.e., electron resonances) at specific energies. Depending on the interaction of the incident electron with a particular atom or molecule and with the surrounding medium, the transient anion can cause desorption of a stable anion and one or many neutral fragments or only neutral particle ejection. The former process occurs when the transitory anionic state dissociates before autoionization whereas, decay by electron emission can, under certain circumstances, results in neutral atom or molecule desorption. Details on these mechanisms will be given at the workshop. They will be illustrated from desorption yield functions recorded by 5-20 eV electron impact on targets ranging from rare gas solid films to more complex ones such as organic thin films.

Th-9:40 "Molecule Adsorbed on Rare-Gas Layers: Electron to Molecule Energy Transfer Mediated by Negative Ion Resonances", C. D. Marinica, D. Teillet-Billy, and J. P. Gauyacq, *Université Paris-Sud and CNRS*^{*}

Chemical reactions at surfaces very often involve a charge transfer as an intermediate step. In particular, it is well known that negative ions as transient species (resonances) play a very important role in surface reactions. Surface processes, such as dissociative adsorption, desorption induced by electronic transition (stimulated by electron or by photon), dissociation and vibrational excitation of adsorbed molecules are very often mediated by molecular negative ions formed by electron capture (1). For such processes mediated by negative ion resonances, the efficiency of the processes is directly linked to the lifetime of the intermediate state and the resonance lifetime strongly depends on the environment of the molecule. This opens the possibility to change the efficiency of a molecular process by tailoring the molecular environment.

We have studied the influence of the local electronic environment on the static properties of the resonance energy position and lifetime and on the dynamics of the electron to molecule energy transfer (vibrational excitation). We have chosen the system formed by an N_2 molecule physisorbed on top of rare-gas layers (Ar or Xe), lying on a metal substrate and studied the well known $N_2^-(^2\Pi_g)$ resonance which is expected to be a very sensitive probe of the local environment. Experimental inelastic electron scattering studies have been performed on this system (2). The present theoretical approach is based on the CAM method which has been previously used to study molecules physisorbed on metal surfaces (3). The rare-gas layer has been modeled as a continuum dielectric medium (4). As expected, the lifetime of the $N_2^-(^2\Pi_g)$ resonance is strongly sensitive to the environment. Due to the electronic confinement at the surface of the dielectric medium, the resonance is stabilized; in the present case with the probe molecule at the surface of the dielectric, the resonance is longer lived than for the free molecule case. This increases lifetime shows up in the vibrational excitation and the signature of this confinement effect appears on the experimental results in (2). This effect is in contrast with the case of a direct adsorption of the molecule on the metal substrate, where the resonance lifetime is shortened. The results, resonance energy position and lifetime, vibrational excitation cross sections, as functions of the rare-gas layer thickness will be presented and discussed at the conference.

(1) L. Sanche, J. Phys. B **23** (1990) 1597; R. E. Palmer and P. Rous, Rev. Mod. Phys. **64** (1992) 383.

(2) M. Michaud and L. Sanche, J. Electron Spectr. Relat. Phenom. **51** (1990) 237; private communication.

(3) V. Djamo, D. Teillet-Billy and J. P. Gauyacq, Phys. Rev. B **51** (1995) 5418.

(4) A. Hotzel, G. Moos, K. Ishioka, M. Wolf and G. Ertl, Appl. Phys. B (1999), in press.

^{*} UMR 8625

Th-10:00 "Absolute Measurement of Total Photo Desorption Yield of Solid Ne in Vacuum Ultraviolet Range", I. Arakawa (1,2) T. Adachi (1), and T. Hirayama (1); (1) *Department of Physics, Gakushuin University*, (2) *Institute for Molecular Science, Okazaki*

Photo-induced desorption at the surface of solid Ne has been investigated. In the present study, "absolute" yield of "total" photo desorption and its excitation energy dependence were measured between 30 nm and 100 nm of the wavelength of the incident light. The sample was a solid Ne film with a thickness between monoatomic layer and 200 atomic layers, which was condensed on a Pt(111) substrate at the temperature of about 6 K. Absolute desorption yield was calculated from the rise of the partial pressure of Ne in a vacuum chamber at the irradiation of the sample by monochromatic light from the synchrotron (UVSOR in IMS, Okazaki) after the careful calibration of the light intensity, the sensitivity of a mass spectrometer, and the pumping speed of pumps.

For a film with a few atomic layers or thinner, the desorption yield is about 1 Ne atom per photon and shows no specific dependence on the excitation energy. In this regime, the Ne film is indirectly excited by the secondary electrons from the substrate. When the film thickness exceeds 10 atomic layers, the peaks caused by the excitonic excitation develop in the desorption spectra. By the excitation of the bulk excitons, the absolute yields reach to almost 1 Ne/photon, while, by the excitation of the surface excitons, they are less than detection limit (0.1 Ne/photon) of the experimental system. Above the band gap energy of solid Ne, the absolute yield has remained almost constant, 1 Ne/photon, and runs up to 2-3 Ne/photon at about twice of the band gap energy.

It can safely be said that the main component in the desorbed species is neutral Ne molecules in the ground state; the absolute yield of metastable desorption at the excitonic excitation is the order of 10^{-3} metastable/photon [1]. The absolute yield of about unity for the total desorption can quantitatively be understood by the following model of desorption. From optical absorption data, the number of excitons created per photon per layer is estimated at about 0.1. The kinetic energies of the particles desorbed through the cavity ejection mechanism is about 0.2 eV and those by the excimer dissociation one 1 eV. Because the cohesive energy of Ne is 0.019 eV, the desorbing particle, which is originated from the 2nd or 3rd layer under the surface after the bulk exciton creation, can blow 10 or more neutral Ne atoms in the overlayer off. The product of these values results in an order of unity of absolute yield of the total desorption.

[1] T. Hirayama et al., *Surf. Sci.* **390**, 266 (1997).

Th-10:50 "Effects of Morphology in Electron-Stimulated Desorption", R. Azria, Y. Le Coat (1), M. Lachgar (1), Michel Tronc (2), L. Parenteau (3), and L. Sanche (3), (1) Université Paris-Sud, (2) Université Pierre et Marie Curie, (3) University of Sherbrooke

In previous electron stimulated desorption experiments from O_2 adsorbed onto different spacer layer films deposited on Pt, at 20K [1], it was shown that the magnitude of the O^- dissociative electron attachment (DEA) yields arising from 0.15 monolayer (ML) of O_2 condensed on a 4 ML spacer films consisting of series of atoms and molecules was strongly influenced by the nature of the atoms or molecules forming the spacer. In the particular case of O_2/H_2O two component targets it was observed that the O^- signal was strongly suppressed. It was noted [1] that the magnitude of the lower O^- DEA yields could be reproduced by an 80% decrease in the lifetime of the dissociative O_2^{-*} ($^2\Pi_u$, $^2\Sigma^+$) resonances with respect to autodetachment, and that the reduction in the lifetime could be due to the local dipole field of the adjacent H_2O molecules.

In this work we have obtained O^- yield functions from 0.1 ML $O_2/4$ ML of different polar molecules (D_2O , ND_3 , CH_3OH , CD_3COOD , CD_3CN) which show that depletion of O^- ESD signal via O_2^{-*} states is not proportional to the dipole moment of molecules forming the spacer layer. In the case of O_2/D_2O target deposited on Pt we have shown by varying the amount of O_2 and the thickness and temperature of formation of the D_2O spacer over wide limits, that the magnitude of O^- yields from DEA is strongly influenced by the morphology of the D_2O spacer (structural state and degree of porosity).

[1] M.A. Huels, L. Parenteau and L. Sanche, *J. Chem. Phys.* 100 (1994) 3940.

Th-11:10 "Giant Cl^- and F^- enhancements in electron-stimulated desorption of CF_2Cl_2 coadsorbed with water or ammonia ices: implications for atmospheric ozone depletion", Q.-B. Lu, and Theodore E. Madey, *Rutgers University*

Dissociative electron attachment can be an important process for the destruction of ozone-depleting chlorofluorocarbons (CFCs) in the upper atmosphere, because of their extremely large electron attachment cross sections. In this study, an electron beam of ~ 250 eV is incident onto a Ru(0001) surface. During electron bombardment, the metal substrate is a source of low-energy secondary electrons which have a maximum yield at 0-2 eV and a high-energy tail that extends 10 eV; low-energy electrons play a dominant role in electron-induced dissociation of CFCs. The yields of negative ions are measured by an electron-stimulated-desorption ion angular distribution (ESDIAD) detector with time-of-flight capability. We have observed giant Cl^- and F^- enhancements by several orders of magnitude in electron-stimulated desorption of a fractional monolayer of CF_2Cl_2 coadsorbed with water ice and ammonia ice on the surface at ~ 25 K, respectively. The enhancement of Cl^- is much stronger than that of F^- , and the enhancements for both ion species by NH_3 coadsorbate are stronger than by H_2O . Moreover, all magnitudes of enhancement increase strongly with decreasing CF_2Cl_2 concentration; for 0.3 ML CF_2Cl_2 , the largest Cl^- enhancements are $\sim 3 \times 10^4$ for NH_3 and $\sim 10^2$ for H_2O . In contrast, the enhancements are much smaller for CF_2Cl_2 coadsorption with nonpolar atoms (rare-gas atoms) or nonpolar molecules (e.g., CH_4 , isoelectronic with H_2O and NH_3). The giant negative-ion enhancements are attributed to dissociation of CF_2Cl_2 by capture of electrons self-trapped (solvated) in polar water or ammonia clusters. This process may be an important sink for chlorofluorocarbons (CFCs) in the atmosphere, where low-energy electrons created by cosmic ray ionization can be trapped in polar stratospheric clouds. Cl^- ions produced may be directly or indirectly converted to Cl atoms, which then destroy ozone.

Th-11:30 "DIET and Reactive Scattering of Low Energy Cations (< 5 eV) in Molecular Surface Ices: Synthesis of New Chemical Species and Small Hydrocarbon Chains Initiated by Low Energy Electron Impact", M. A. Huels, L. Parenteau, and L. Sanche, *University of Sherbrooke*

The subsequent interactions of low energy secondary electrons and ions, formed during radiolysis of solid or liquid media, with atoms and molecules have received renewed attention in the recent past; this is mainly due to the fact that they play an important role in the chemical degradation and/or transformation of dielectric solids and thin films, as well as the synthesis of more complex chemical species from stable, less complex, naturally occurring components. Thus, it is not surprising that the contexts where such secondary electron and ion reactions occur are those wherever ionizing radiation deposits energy in matter, and range from damage to cellular DNA during tumor radiotherapy, to the synthesis of new, or more complex (sometimes organic) molecules at the surfaces of extraterrestrial icy grains or particles, or icy regions of some planets and their satellites, which are exposed to various space radiations.

Here we present results of cation scattering in, and desorption from, molecular ices initiated by low energy electron (<40 eV) impact, *viz.* DIET. The thin ice layers studied here consist of ca. 5 monolayer thick binary mixtures of various small molecules such as $^{16}\text{O}_2$, $^{18}\text{O}_2$, N_2 , CO, and CH_4 , condensed at 20K under UHV conditions. The samples are irradiated directly with a low energy ($E_0 \leq 40$ eV) electron beam emanating from a hemispherical monochromator ($\Delta E_0 \approx 80$ meV), and desorbing ionic species are mass selected with a high resolution mass spectrometer, and detected using standard charge sensitive electronics.

For CO/ N_2 ices, reactions of C^+ (<4 eV) with N_2 or CO lead to formation and desorption of CN^+ , and C_2^+ , respectively, whereas for O_2/N_2 , and N_2/CH_4 solids, cation reactions result in NO^+ and NH^+ desorption, respectively. For $^{18}\text{O}_2/\text{N}_2/^{16}\text{O}$, and $^{18}\text{O}_2/^{16}\text{O}_2$ films we also observe O- and/or N-atom abstraction. For O_2/CH_4 solids, reactions of low energy O^+ , with surface kinetic energies in the laboratory frame of less than 5 eV, lead to formation and desorption of OH^+ , H_2O^+ , H_3O^+ (hydronium), OCH^+ , OCH_3^+ , and very small quantities of OCH_2^+ (formaldehyde). For pure CH_4 solids, reactions of CH_n^+ fragments with CH_4 lead to desorption of CH_4^+ , CH_5^+ , C_2H_3^+ , and C_2H_5^+ , and small traces of C_2H_2^+ (acetylene or vinylidene) and C_2H_4^+ (ethylene). Our measurements suggest that the more intense carbon chains with odd numbers of hydrogens are formed in surface reactions of CH_3^+ , and C_2H_5^+ , whereas those with even numbers of hydrogens are the result of CH_2^+ reactions with CH_4 . We will discuss the results within the context of previous and current measurements of anion (mainly O^-) reactions in organic surface ices, consisting of linear and cyclic hydrocarbons, which lead to atom-, and functional group exchange, charge transfer, hydrogen abstraction, and reactive charge transfer. Our results indicate that secondary electrons, formed at or within icy surface layers by ionizing space radiations, can initiate various subsequent ion reactions which result in the synthesis of new, more complex, organic chemical species.

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THURSDAY SEPTEMBER 30

AFTERNOON

SESSION ThA1 - Chair, E. Malcolm Williams

- 1:20 **INVITED - Ion Desorption Induced by Core-Electron Transitions Studied with Electron-Ion Coincidence Spectroscopy**
K. Mase, *Institute for Molecular Science, Okazaki*
- 2:00 **Photo-Stimulated Ion Desorption from TiO₂ (110) Surface**
S. Tanaka, K. Mase, M. Nagasono, and M. Kamada, *Institute for Molecular Science, Okazaki*
- 2:20 **Energy Space Density Space Dynamics of DIET and DIMET Processes**
H. Guo, *University of New Mexico*
- 2:40 **DIET of Biological Molecular Systems Chemisorbed onto a Surface**
H. Abdoul-Carime, P. C. Dugal, and L. Sanche, *Université de Sherbrooke*

3:00 -COFFEE BREAK-

SESSION ThA2 - Chair, Katsumi Tanimura

- 3:30 **AFM and Time-Of-Flight Studies of Electron-Stimulated Desorption Processes in Bulk Single Crystals and Thin Epitaxial Layers of Alkali Halides**
M. Szymonski, B. Such, P. Struski, J. Kolodziej, P. Czuba, and P. Piatkowski, *Jagiellonian University*
- 3:50 **New Insight into Potential Sputtering of Insulators**
G. Hayderer, C. Lemell, L. Wirtz, M. Schmid, J. Burgdörfer, P. Varga, H. P. Winter and F. Aumayr, *TU Wien (Vienna University of Technology)*
- 4:10 **Observation of Surface Modification Induced by Bombardment of Highly Charged Ions**
R. Minniti, L. P. Ratliff, and J. D. Gillaspay, *NIST*
- 4:30 **Electron Stimulated Desorption of Hydrogen and Deuterium from Silicon (111) Surfaces Detected by Second Harmonic Generation**
M. Albert, G. Luepke, N. Tolk, *Vanderbilt University*
- 4:50 **Laser Induced Desorption from Metals**
D. P. Taylor and H. Helvajian, *The Aerospace Corporation*
- 5:10 **Desorption and Ablation of Diamond by Ultra-Short Laser Radiation**
V. Schmidt (1), W. Husinsky (1), Z. Marka (2), G. Betz (1), and N. Tolk (1, 2);
(1) *Vienna University of Technology*, (2) *Vanderbilt University*

6:00 -DINNER-

7:30 - 9:30 - POSTER SESSION-

Th-1:20 INVITED - "Ion Desorption Induced by Core-Electron Transitions Studied with Electron-Ion Coincidence Spectroscopy", K. Mase, Institute for Molecular Science, Okazaki

Energy-selected electron ion coincidence (EICO) spectroscopy combined with synchrotron radiation is an ideal tool for investigations of the ion desorption induced by core-electron transitions, because it provides ion mass spectra for the ion desorption channels related to the selected electron transitions [1, 2]. We have developed an EICO apparatus, which consists of a cylindrical mirror electron energy analyzer and a time-of-flight ion mass spectrometer [1,3]. A photoelectron-photoion coincidence (PEPICO) investigation of condensed $\text{SiF}_3\text{CH}_2\text{CH}_2\text{Si}(\text{CH}_3)_3$ provided a direct evidence of site-specific ion fragmentation induced by core-electron excitations, that is, the ion species is different for different Si:2p core-electron ionizations [4]. A PEPICO study of a fluorine-saturated Si(111) surface showed that Si:2p ionization at SiF, SiF₂, and SiF₃ sites are responsible for F⁺ desorption [2]. An Auger electron photoion coincidence (AEPICO) study of condensed H₂O, on the other hand, demonstrated that H⁺ desorption is stimulated by Auger processes leaving two-hole states [5]. Furthermore, the ion desorption probabilities are found to depend on the bonding character of the orbitals where holes are created and the effective hole-hole Coulomb repulsion. AEPICO investigations of H⁺ desorption induced by resonant core-electron excitations of condensed H₂O clearly showed that one-electron-one-core-hole state or one-electron-two-valence-hole states are responsible for the H⁺ desorption mechanism [6]. An AEPICO study of H₂O dissociatively chemisorbed on a Si(100) surface showed that the lifetime of the excited electron is too short to enhance the H⁺ desorption probability, and that multi-hole states (more than two holes) are responsible for the H⁺ desorption [7]. A recent AEPICO study of CaF₂(111) film presented a direct evidence of F⁺ desorption induced by F1s surface core-exciton [2, 8]. These investigations demonstrate that EICO spectroscopy is a novel and powerful tool in DIET.

- [1] K. Mase, M. Nagasono, S. Tanaka, J. Electron Spectros. Relat. Phenom., in press.
- [2] K. Mase and S. Tanaka, Jpn. J. Appl. Phys., in press.
- [3] K. Mase et al., Rev. Sci. Inst. 68, 1703 (1997).
- [4] S. Nagaoka et al., J. Chem. Phys. 107, 10751 (1997).
- [5] M. Nagasono et al., Chem. Phys. Lett. in press.
- [6] K. Mase et al., Surface Sci. 390, 97 (1997); K. Mase et al., J. Chem. Phys. 108, 6550 (1998).
- [7] S. Tanaka et al., Surface Sci. 390, 204 (1997).
- [8] S. Tanaka et al., J. Electron Spectros. Related Phenom. 92, 119 (1998).

Th-2:00 "Photo-Stimulated Ion Desorption from TiO₂ (110) Surface", S. Tanaka, K. Mase, M. Nagasono, and M. Kamada, *Institute for Molecular Science, Okazaki*

The mechanism of photo-stimulated ion desorption from the TiO₂(110) surface has been investigated by the use of synchrotron radiation and the electron-ion coincidence spectroscopy. The photoelectron-photoion coincidence (PEPICO) spectra were obtained by measuring the time between the detection of desorbed ions and that of photoelectrons excited from the core- and valence-levels. The Auger electron-photoelectron spectra were obtained by measuring the time between the detection of ions and that of Auger electrons. TiO₂(110) surface was cleaned by several cycles of Ar⁺ sputtering and heating. In order to avoid the oxygen vacancy on the surface, it was heated in oxygen of 10⁻⁶ Torr just before every measurement. In PEPICO measurements for TiO₂(110), clear coincidence was observed between the desorption of oxygen ions and the photoelectrons from the O-1s, Ti-2s, Ti-2p, Ti-3s and Ti-3p levels, meanwhile, no coincidence was observed for valence (mainly O-2p) and O-2s levels. In AEPICO measurements, the coincidence with the oxygen ion desorption was observed for the O-KL₁L₁, O-KL₁V and Ti-LMM Auger electrons, while it was small for the O-KVV and Ti-LVV Auger electrons. These results indicate the following conclusions; 1) the oxygen ion desorption from the TiO₂(110) surface is induced by the excitation and decay of core levels at Ti and O atoms, 2) the normal Auger decay which creates two holes at the valence level does not yield the ion desorption, while the Auger decay processes which create holes at deeper levels and/or the double Auger process are responsible for the oxygen ion desorption.

Th-2:20 "Energy Space Density Space Dynamics of DIET and DIMET Processes", H. Guo, *University of New Mexico*

DIET/DIMET events on solid surfaces are dissipative processes, which can be described quantum mechanically by the Liouville-von Neumann equation. We discuss an application of a newly proposed density operator propagation scheme to photon-stimulated desorption (PSD) dynamics. The discretization of the density operator is carried out in the energy representation where the basis consists of the eigenfunctions of a modified system Hamiltonian. Such energy space discretization provides a minimal basis size in solving the Liouville-von Neumann equation and ease in extracting the dynamic information. Both MGR- and Antoniewicz-type desorption schemes are examined in both single and multiple excitation regimes. For one-dimensional models pertaining to the PSD of NO from metals, the observables such as the desorption yield and product kinetic energy distribution cannot differentiate the two desorption mechanisms.

**Th-2:40 "DIET of Biological Molecular Systems Chemisorbed onto a Surface",
H. Abdoul-Carime, P. C. Dugal, and L. Sanche, *Université de Sherbrooke***

For more than half century, many studies have been devoted to the understanding of alteration of biological cells induced by high energy radiation (X-rays, UV,...). Genetic damage can involve the action of reactive free radicals, solvated electrons and secondary low energy electrons ($< 30\text{eV}$) which are generated along the ionisation track. Up to now, most of experimental studies focused on the DNA degradation induced by free radicals and solvated electrons, but the effects of secondary electrons are still unknown.

Recently, many experimental efforts have been devoted to isolate cellular components from their environment and therefore allowed fundamental studies of alteration of biological molecules by slow electrons[1-3]. Low Energy Electron (0-30eV) Stimulated Desorption of neutral fragments experiment [4] coupled to the Self-Assembled Monolayer technique [5] for oligonucleotides chemisorbed onto a metal substrate has been used to investigate the effects of secondary electron damage in small sequence of a DNA single strand. We have shown that under electron impact, dissociation of DNA bases occurs leading to the production of CN, OCN and/or H_2NCN neutral species which are presently the most intense observable yields [3,6]. The incident electron energy dependencies of these desorbed neutral species exhibit typical signatures of dissociative electron attachment (DEA) process initiated by the formation of shape and core excited resonances. Moreover, the neutral species production is shown to be strongly influenced by the nature of the DNA bases and the base composition involved in the oligonucleotide. For instance, substitution of thymine by bromouracil increases the production of neutral fragments by as much as a factor of about 3 for the 9-30eV electron energy range. These results will be presented and discussed at the workshop.

1. C. Desfrancois, H. Abdoul-Carime, C. P. Schulz, J.P.Schermann, *Science*, **269**, (1995)
2. M. A.Huels, I. Hahndorf, E. Illenberger, L. Sanche, *J.Chem.Phys*, **108**, 1309, (1998)
3. P. C. Dugal, M. A. Huels, L. Sanche, *Radiation Research*, **151**, 325, (1999)
4. L. Sanche, *Scanning Microscopy*, **9**(3), 619, (1995)
5. C. E Rabbe-Clemmer, A. J. Leavitt, T. P. Beebe Jr, *Langmuir*, **10**, 1796, (1994)
6. H. Abdoul-Carime, P. C. Dugal, L. Sanche, *Radiation Research*, accepted for publication

Th-3:30 "AFM and Time-Of-Flight Studies of Electron-Stimulated Desorption Processes in Bulk Single Crystals and Thin Epitaxial Layers of Alkali Halides",
M. Szymonski, B. Such, P. Struski, J. Kolodziej, P. Czuba, and P. Piatkowski,
Jagiellonian University

Electron-stimulated desorption (ESD) of KCl (001) and KBr (001) epitaxial thin films and bulk single crystals due to 1 keV electron bombardment was investigated in UHV by means of a non-contact atomic force microscopy (NC-AFM) and a mass-selected time-of-flight spectroscopy (TOF). There were two basic kinds of structures visible on the irradiated surfaces. The first one consisted of rectangular holes of monolayer depth with edges oriented along the main crystallographic directions of the (001) plane. Spots agglomerated mostly at the edges formed the second characteristic kind of the observed structures. Dependence of the structure size and density was measured as a function of the electron dose and the sample temperature. We found that ESD of both alkali halides studied in this work essentially occurred in layer-by-layer mode, except for the fact that the erosion of the consecutive layer started before the erosion of the previous one was completed. The average desorption rate was determined quantitatively from our microscopic data and they were compared with the ones obtained from thin film removal experiments. The analysis of our AFM images obtained for various doses of electrons allowed us for studying a dependence of the local desorption yield on the actual topography of the imaged area. Furthermore a correlation between the relative contribution of the two desorption components (thermal and non-thermal), as determined with TOF, and the corresponding surface topographies imaged with NC-AFM was observed for various temperatures of the samples. Consequently, a comprehensive description of the observed desorption features will be presented.

Th-3:50 "New Insight into Potential Sputtering of Insulators", G. Hayderer, C. Lemell, L. Wirtz, M. Schmid, J. Burgdörfer, P. Varga, H.P. Winter and F. Aumayr, TU Wien (Vienna University of Technology)

In recent studies on the impact of slow multiply charged ions on insulator surfaces, a dramatic increase of the yields for sputtering and secondary ion emission with projectile charge state has been observed for certain target species (e.g., for LiF and SiO₂) [1]. In contrast to the well established kinetic sputtering, the ejection of target atoms and ions due to the potential energy of ions is still largely unexplored. Currently available experimental evidence and theoretical considerations strongly favour a so-called "defect-mediated desorption" model over an explanation involving a "Coulomb explosion" mechanism. To gain more insight into the mechanisms responsible for potential sputtering (PS) we have measured total sputtering yields of LiF under impact of slow (20 eV, 100 eV, 500 eV and 1000 eV kinetic energy) singly charged ions. In these experiments the available potential energy has been varied from 5.1 eV (Na⁺) to 24.6 eV (He⁺) and its influence on PS was investigated. Below 10 eV potential energy, sputtering can only be observed for sufficiently fast projectiles (500 eV and 1000 eV) and is therefore ascribed to transfer of kinetic energy. The minimum potential energy necessary to induce PS from LiF was determined to be about 10 eV. This coincides with the energy required to produce a "cold hole" in the F-valence band of LiF by resonant neutralization. At about 20 eV potential energy Auger capture becomes possible. The resulting electron-hole pairs localize as self-trapped excitons leading to a further increase in the sputtering yield. We carry out comparison with model calculations and present evidence for the two mechanisms.

[1] M. Sporn, et al., Phys. Rev. Lett. **79**, 945 (1997).

Th-4:10 "Observation of Surface Modification Induced by Bombardment of Highly Charged Ions", R. Minniti, L. P. Ratliff, and J. D. Gillaspy, *NIST*

A highly charged ion (HCI) can store large amounts of internal potential energy, (e.g., 54000 eV for a Xe^{44+} ion). During the interaction of a HCI with a solid surface this available energy can be transferred by neutralizing the charge of the ion, which can result in surface modification. We have exposed surfaces of highly oriented pyrolytic graphite to a beam of xenon highly charged ions. Following the exposure the surfaces were imaged in-situ using a scanning tunneling microscope. We observe nanometer scale features on the surface that correspond to single ion impacts up to 10 nm in diameter. The dependence of the size of the ion induced nanoscale features with potential energy of the ion will be discussed.

Th-4:30 "Electron Stimulated Desorption of Hydrogen and Deuterium from Silicon (111) Surfaces Detected by Second Harmonic Generation", M. Albert, G. Luepke, N. Tolk, *Vanderbilt University*

Second Harmonic Generation (SHG) provides a sensitive probe of the quantity of Hydrogen or Deuterium remaining on a Silicon surface. With fraction-of-a-monolayer sensitivity, lower energy processes which do not result in ionized desorption can be easily observed. Using this technique we have measured electron stimulated desorption of Hydrogen and Deuterium from a well prepared Silicon (111) surface. With simple modeling we have determined the total absolute cross-section for several incident energies and thresholds have been observed. This work is funded by the Office of Naval Research.

Th-4:50 "Laser Induced Desorption from Metals", D. P. Taylor and H. Helvajian, *The Aerospace Corporation*

It has now been a decade since Welle and Helvajian reported high kinetic energy silver ions in a UV laser induced desorption (LID) experiment on silver. The LID process leading to high kinetic energy ions from metal surfaces has most often been explained in terms of the Ritchie surface plasmon theoretical model. Although this model is widely accepted, the weight of supporting evidence is not very compelling. So far, the best experimental support for the surface plasmon model for LID is provided by Shea and Compton (PRB 47, 9967, (1993)). In an experiment on a roughened silver sample, they observed silver ions with the kinetic energy of the surface plasmon. We will present the results of our recent LID experiments and some related material.

Th-5:10 "Desorption and Ablation of Diamond by Ultra-Short Laser Radiation",
V. Schmidt (1), W. Husinsky (1), Z. Marka (2), G. Betz (1), and N. Tolk (1, 2); (1)
Vienna University of Technology, (2) Vanderbilt University

We have studied the desorption and ablation process from thin diamond. Polycrystalline films on Si- (10 μm thick) and Mo- (40 μm) substrates and a free standing polycrystalline diamond film (400 μm) have been investigated. The main emphasis of these studies was to identify the initial steps leading to the ablation process for ultra-short laser pulses. We have used 20 fsec pulses from Ti:Sapphire Femto-Laser-System (central wavelength around 800 nm) the radiation a Free Electron Laser (Vanderbilt FEL) (1 psec long micro-pulses; 3.5, 3.7 and 5 μm).

We have measured the mass spectrum of positive ionic species desorbed for various parameters of the laser radiation with a TOF spectrometer. In order to obtain a reasonably systematic picture, thresholds and mass spectra were measured as a function of the number of laser shots an "originally virgin spot" on the target had been exposed to. In the case of the FEL, one shot, however, corresponds to one macro-pulse which itself consists of several 350 psec spaced micro-pulses. The length of the macro-pulses was approximately 4 μsec . Distinct thresholds for desorption have been observed. Macroscopic evaluation of areas hit by the laser beam show distinct differences for the FEL radiation and the femto-laser. In the case of the FEL craters and holes can be observed, while the absolute amount of material removed by the femto radiation is much smaller. Some of these wavelengths correspond to maxima in the absorbency due to H-adsorbate vibrations and a bulk two-phonon resonance. Other wavelengths do not correspond to any known absorption maximum. A comparison of the ablation behavior, therefore, can yield important information about the first step of the desorption/ablation process itself. The diamond films (virgin spots and region where ablation had occurred) were characterized by micro-Raman spectroscopy after exposure.

FRIDAY OCTOBER 1

MORNING

SESSION FrM1 - Chair, Marek Szymonski

- 9:00 **INVITED - Desorption Induced by Electronic Transitions of Alkali Metal Atoms and Oligomers from the Surface of Superfluid Liquid Helium Droplets**
G. Scoles, *Princeton University*
- 9:40 **DIET of Metastable Kr* Atoms via Electron Resonances in Kr/Ar Alloy Films**
A. D. Bass, E. Vichnevetski and L. Sanche, *Université de Sherbrooke*
- 10:00 **Electron-Stimulated Desorption of K and I from KI(100): Yields, Threshold Energies, and Velocity Distributions**
A. Alexandrov(1), M. T. Sieger(1), R. G. Tonkyn(1), T. M. Orlando, N. Zema(2), and M. Piacentini(3); (1) *Pacific Northwest National Laboratory*, (2) *CNR*, (3) *Universita di Roma*

10:20 -COFFEE BREAK-

SESSION FrM2 - Chair, Robert A. Bartynski

- 10:50 **INVITED - Surface Transition State Spectroscopy: Femtosecond Dynamics of Photodesorption of Cs from Copper**
H. Petek, *Hitachi, Japan*
- 11:10 **Laser-Induced Electronic Bond Breaking and Desorption of Constituent Atoms on InP(110)-(1x1)**
Jun'ichi Kanasaki, Noriaki Mikasa, Shinsuke Kotake, and Katsumi Tanimura, *Nagoya University*
- 11:30 **Time-Resolved Femtosecond Laser Induced Desorption from Magnesium Oxide and Lithium Fluoride Single Crystals**
Alan G. Joly, Kenneth M. Beck, and Wayne P. Hess, *Pacific Northwest National Laboratory*

12:00 -LUNCH-

1:00 DEPARTURE

Fr-9:00 INVITED - "Desorption Induced by Electronic Transitions of Alkali Metal Atoms and Oligomers from the Surface of Superfluid Liquid Helium Droplets", G. Scoles, Princeton University

Helium droplet isolation spectroscopy is a relatively new technique in which a very cold (0.4K) beam of liquid He droplets (each containing about 10^4 atoms) is used to capture in a pick-up cell one or more atoms or molecules which are then probed downstream by laser induced fluorescence or beam depletion spectroscopy. If the trapped species have a very low ionization potential (i.e., very long decay range of their electronic wavefunction) they interact very weakly with the He host matrix, are not solvated and reside on the surface of the droplet. Upon electronic excitation these surface species may undergo several processes which can be studied by frequency resolved or time resolved spectroscopy. We will report on a series of experiments in which sodium atoms bound to the helium surface experience desorption after being electronically excited in the neighborhood of their $p \leftarrow s$ transition. Two processes can be distinguished. If a Σ type orbital is formed in the excited state the Na atoms undergo sudden evaporation and emit from the gas phase. If, instead, a Π type orbital is created, a $\text{Na}^* \text{He}$ exciplex may form in a time which depends on whether the transition occurs to the $1/2$ or $3/2$ spin orbit state of the excited complex and which has been measured by time-correlated single photon counting. A theoretical discussion of the process shall clarify why only one He atom joins the excited Na atom to form the exciplex (as opposed to several atoms as it occurs when the Na atoms are excited in bulk liquid He) and why the lower spin orbit excimer rate of formation is more than one order of magnitude smaller than for the higher spin orbit case. Time-resolved studies shall also be discussed in which we exploit the selective survival of high spin (van der Waals bound) oligomers formed on the surface of the droplet over their low spin (chemically bound) counterparts which are blown off the cluster surface by the vibrational relaxation that immediately follows their formation. The latter evaporation process, which, contrary to the previous ones, occurs on the ground state potential energy surface, can also be studied by laser induced fluorescence spectroscopy because the evaporation of the freshly formed molecules from the very cold He surface leads to very low transversal velocities so that the evaporated molecules do not disperse and travel in the same forward direction as the main beam.

(1) Work carried out in collaboration with James Reho, John Higgins, Carlo Callegari and Kevin Lehmann with the sponsorship of AFOSR.

Fr-9:40 "DIET of Metastable Kr* Atoms via Electron Resonances in Kr/Ar Alloy Films", A. D. Bass, E. Vichnevetski and L. Sanche, *Université de Sherbrooke*

Excitation pathways within rare gas solids have been [1] and remain an active area of theoretical and experimental investigation [2,3,4] since this group of materials present conceptually simple models for dielectric and semi-conductor behaviors. Numerous techniques have been employed to study excitation within these materials and much information has been gained from measurements of the DIET of excited particle from thin rare gas films [2]. In general for excitation at energies lower than the band gap, desorption is correlated to exciton formation and trapping. Below the threshold of the $n=2$ bulk and surface excitons, atomic desorption proceeds via the cavity expulsion mechanism. Recently [5], we have shown that electron-impact excitation of the electron-exciton complex or 2P Ar $^-$ resonance of solid Ar [6] can lead to the desorption of metastable Ar* atoms even though the resonance energy of ~ 11.5 eV lies below the threshold for exciton formation. Such 'sub-threshold' desorption can occur only when the Ar $^-$ is able to transfer its surplus electron into a vacant sub-vacuum electronic state of either the substrate onto [5] or of a suitable dopant [7]. In this work we demonstrate that under electron impact the desorption of metastable Kr* atoms from Ar/Kr alloy films is observed at 10 eV, i.e., below the energy of the lowest exciton states of the alloy. The data indicate that desorption at this energy requires that Kr atoms be in close proximity to the Pt substrate and suggests the involvement of a Kr electron-exciton complex. Time of flight measurements provide further information on the dynamics of this process.

[1] N. Schwenter, E-E. Koch and J. Jortner, *Electronic excitations in condensed rare gases*, (Springer-Verlag Berlin 1985)

[2] G. Zimmerer, *Nuc. Instrum and Methods B*. 91, 601 (1994)

Fr-10:00 "Electron-Stimulated Desorption of K and I from KI(100): Yields, Threshold Energies, and Velocity Distributions", A. Alexandrov (1) M. T. Sieger (1), R. G. Tonkyn(1), T. M. Orlando, N. Zema (2), and M. Piacentini(3); (1) *Pacific Northwest National Laboratory*, (2) *CNR*, (3) *Universita di Roma*

We have studied the low-energy (5-100 eV) electron-stimulated desorption (ESD) of neutral K and I fragments from KI(100) single crystals using quadrupole and time-of-flight mass spectrometry. In the latter case, detection schemes using laser resonance-enhanced multiphoton ionization (REMPI) were used. Thresholds measurements, which were obtained at elevated temperatures (425 K) to reduce complications from surface charging, indicate a weak onset of K and I desorption near approximately 6 eV. This threshold is close to the first exciton band and is consistent with previous PSD measurements [N. Zema, et. al. *Phys. Rev.B*, **55**, 5448 (1997)] which demonstrate the importance of excitons in the PSD of alkali halides. A stronger ESD threshold for both K and I is observed at about 10 eV which is near the lowest valence-to-conduction band transition. The time-of-flight (TOF) distributions of K are thermal whereas the TOF distributions of I are bi-modal with a substantial non-thermal component. The intensity of this non-thermal component is very weakly dependent upon the substrate temperature, whereas the intensity of the thermal component increases significantly with temperature. The temperature dependent studies indicate that the thermal component results from decay of diffusing H-centers. The temperature and dose dependence of the non-thermal component implies that this may involve a two step process. REMPI results have been obtained for the I(3/2) state and experiments are underway utilizing REMPI transitions which detect the I(1/2) level. These measurements will allow us to check for spin-effects in the desorption dynamics.

Fr-10:50 INVITED - "Surface Transition State Spectroscopy: Femtosecond Dynamics of Photodesorption of Cs from Copper", H. Petek, Hitachi, Japan

Observation and manipulation of transition states in chemical reactions is one of the ultimate goals in chemistry. This dream has been realized for simple chemical reactions in the gas phase where the quantum mechanical phase and energy relaxation in the course of reaction can be resolved by the currently available ultrafast laser techniques. However, most chemical reactions of significant practical importance occur in the condensed phase and at interfaces between materials, where ultrafast relaxation processes often present insurmountable difficulties for the direct probing of the transition states. However, the recent observation of the time evolution of the Cs anti-bonding state on the Cu(111) surface in the process of desorption, shows that there may be fortunate cases where the reactant bonding and electronic band structure may be favorable to observation of transition states even on metal surfaces [1]. Interferometric time-resolved two-photon photoemission [2, 3] measurements of Cs atoms on single crystal copper surfaces show a strong correlation between the adsorbate/substrate binding and the excited state lifetime. The electronic relaxation of Cs on Cu(110) and Cu(100) is too fast to resolve; however, on Cu(111) the phase and energy relaxation are 15 and ~50 fs, respectively. This is sufficiently slow to observe the time evolution of the transition state in photodesorption of Cs atoms. The interferometric measurements indicate that the excitation of Cs atoms occurs by direct substrate-to-adsorbate photoexcitation, rather than through the conventional hot-electron mechanism, which is often used to describe DIET processes [4].

- 1 S. Ogawa, H. Nagano, and H. Petek, Phys. Rev. Lett. 82, 1931 (1999).
- 2 S. Ogawa, et al., Phys. Rev. Lett. 78, 1339 (1997).
- 3 H. Petek and S. Ogawa, Prog. Surf. Sci. 56, 239 (1997).
- 4 F. Weik, A. d. Meijere, and E. Hasselbrink, J. Chem. Phys. 99, 682

Fr-11:10 "Laser-Induced Electronic Bond Breaking and Desorption of Constituent Atoms on InP(110)-(1x1)" Jun'ichi Kanasaki, Noriaki Mikasa, Shinsuke Kotake, and Katsumi Tanimura, *Nagoya University*

Clean surfaces of InP(110)-(1x1) with well-developed wide terraces were excited with ns-laser pulses, photon energies of which (2.6-3.0 eV) fall in resonance to the surface transitions. The induced changes in surface-atomic structure were studied by scanning tunneling microscopy (STM), and desorption of constituent atoms were studied by means of non-resonant multiple photoionization (NRMPI) spectroscopy with femtosecond laser pulses. STM observation yields direct atomic imaging of the induced changes, while NRMPI enables us to detect simultaneously all neutral desorbed species with sensitivities as high as 10^{-7} monolayer per pulse.

STM studies have demonstrated for the first time that P and In atoms at intrinsic surface sites of (1x1) structure are removed by purely electronic processes. An interesting feature revealed is efficient formation of vacancy strings at P sites elongated along $[1\bar{1}0]$ -chain direction, together with formation of single P vacancies. Analysis of the formation yield of P-vacancy strings as functions of dose and excitation intensity has shown that the string formation is due to successive and preferential removal of P atoms located at nearest neighbor sites of P vacancies. On the other hand, In vacancies are mostly in the form of single vacancy, and the total yield is less than that of P vacancies. Although the resulted configurations of the vacancies are different, the efficiencies of bond breaking of both atoms show strong superlinear dependence on excitation intensity, suggesting strongly non-linear localization of surface excited species. In fact, the two-hole localization model describes satisfactorily the superlinear dependence for both P and In vacancy formation.

Femtosecond MPIS studies have shown that P and In atoms, together with P_2 molecules, are desorbed upon surface excitation, with the largest yield of P atoms. The yields of these species show superlinear dependence on the excitation intensity, similarly to the bond breaking efficiencies. Time-of Flight measurements of the desorbed species show that the most probable translational energies of P and In atoms are 0.45 and 0.94 eV, respectively. In view of the results of STM studies on the irradiated surface, we ascribe the desorption of single P and In atoms to the direct consequence of the electronic bond breaking of the constituent atoms. Quantitative analysis of the yields of P_2 molecules desorbed and of STM-revealed excitation-induced adatoms on the surface have shown that the desorption of P_2 takes place at surface adatoms as the precursor.

Fr-11:30 "Time-Resolved Femtosecond Laser Induced Desorption from Magnesium Oxide and Lithium Fluoride Single Crystals", Alan G. Joly, Kenneth M. Beck, and Wayne P. Hess, *Pacific Northwest National Laboratory*

We have used the pump-probe technique to measure the positive ion yield, from MgO and LiF single crystals, as a function of time-delay between two sub-threshold UV femtosecond laser pulses and compare the ion desorption processes between these two wide-gap materials. We find that the ion yield from MgO depends critically on the laser pulse delay, Δt . At zero pulse delay, $\Delta t = 0$, the (single pulse condition) excitation of MgO produces a variety of ions such as Mg^+ , H^+ , MgO^+ , and impurity ions. In contrast, a pulse delay of only $\Delta t = 500$ femtoseconds drastically alters the ion yields and nearly eliminates desorption for all ions but Mg^+ . The use of a pair of delayed femtosecond laser pulses can thus influence the type and abundance of desorbed ions. The time-resolved Mg^+ desorption yield displays a short-time decay, in the 10's of picoseconds range, and a persistent longer-time decay extending over 100's of picoseconds. The short-time decay lifetime is of similar duration as the conduction band electron lifetime in MgO. The yield decrease observed for H^+ , and other impurity ions, for pulse delays greater than $\Delta t = 500$ femtoseconds, indicates that direct multiphoton processes may be important for desorption of these species. We also detect Li^+ desorption from LiF single crystals following two-pulse femtosecond excitation. Again, the ion yield may be drastically altered depending on the pulse delay with a large Li^+ desorption yield observed at short pulse delays. The ion desorption thresholds and fluence versus yield dependencies were characterized following both femtosecond and nanosecond UV laser irradiation. The observed thresholds are similar and suggest, that although the ion desorption mechanism is dominated by defect photoabsorption, significant conduction band electron generation may contribute to the desorption mechanism following femtosecond excitation. We hypothesize that the femtosecond laser desorption mechanism, in MgO at least, is enhanced by the creation of electron hole pairs through nonresonant two-photon excitation. At low fluence, sub-bandgap nanosecond pulses cannot produce conduction band (CB) electrons of sufficient quantity to broadly influence laser desorption. However, for ultrafast excitation, pulse intensities are greater by a factor of 10^3 to 10^4 and the production rate of CB electrons is increased by six to eight orders of magnitude. Under this scenario it is likely that a high degree of electronic excitation could exist during and immediately following the femtosecond pulse. On the basis of calculations we conclude that significant CB densities of $\sim 10^{17}$ CB e-/cm³ may exist following 265 nm femtosecond excitation of MgO. The observed differences in ion desorption threshold and fluence dependence between nanosecond and femtosecond laser sources clearly indicates that short pulse excitation explores new aspects of laser/solid interactions.

Poster Presentations

** Competing for Student Award

1. **Electron-Stimulated Desorption of Lithium Atoms from Oxidized Molybdenum Surfaces**
V. N. Ageev (1), Yu. A. Kuznetsov (1), and T. E. Madey (2); (1) *A. F. Ioffe Institute, St. Petersburg, Russia*, (2) *Rutgers University*
2. **Electron-Stimulated Desorption of Lithium Ions from Silicided Tantalum Surfaces,**
V. N. Ageev and S. M. Solovev, *A. F. Ioffe Institute, St. Petersburg, Russia*
3. **ESD and PSD of Alkalis from Oxide Surfaces - Relevance to Tenuous Planetary Atmospheres**
B. V. Yakshinskiy and Theodore E. Madey, *Rutgers University*
4. **Low-Temperature Water Ice Phases Probed by Electron Stimulated Desorption**
T. M. Orlando, M. T. Sieger and W. R. Wiley, *Pacific Northwest National Laboratory*
5. **Electron-Induced Processes in Condensed Films of CF_2Cl_2**
M. N. Hedhili (1), Q. B. Lu (1), T. E. Madey (1), M. Lachgar (2), Y. Le Coat (2), R. Azria (2), and M. Tronc(3); (1) *Rutgers University*, (2) *Université Pierre et Marie Curie*, (3) *Université Paris-Sud*
6. **Photon Stimulated Ion Desorption of Poly-Methylmethacrylate and Poly-Isopropenylacetate Thin Films following Oxygen Core Excitation**
K. Fujii** , S. Wada, D. Taga, Y. Nakashima, T. Sekitani and K. Tanaka, *Hiroshima University*; M. Tooyama, *Mitsubishi Rayon Co., Ltd., Otake, Japan*
7. **A Study of Photon Induced Processes with Adsorption-Desorption of Glycine at the $\text{TiO}_2(110) (1 \times 2)$ Surface**
E. Soria (1), I. Inmaculada (2), E. Roman (3), E.M. Williams (4), and J.L. de Segovia (1); (1) *CETEF "L. Torres Quevedo"*, (2) *Universidad Carlos III*, (3) *CSIC*, (4) *The University of Liverpool*
8. **Time-Of-Flight Techniques for the Investigation of Kinetic Energy Distributions of Ions and Neutrals Desorbed by Core Excitations**
R. Weimar (1), R. Romberg (1), S. Frigo (2), B. Kassuehlke (1), and P. Feulner (1); (1) *Technische Universität München*, (2) *Advanced Photon Source, Argonne*
9. **PSD of Neutral Hydrogen Atoms from Condensed Water and Ammonia by Resonant O1s and N1s Excitation: Search for the Signature of Ultrafast Bond Breaking**
R. Romberg** , S. Frigo (1), A. Ogurtsov (2), P. Feulner, and D. Menzel, *Technische Universität München*; (1) *Advanced Photon Source*, (2) *Verkin Institute for Low Temperature Physics & Engineering, Kharkov, Ukraine*
10. **A New Analyser for Gas and Ion Analysis: The Splat Analyser**
Robert G. Jones and N.E. Abrams, *University of Nottingham*

11. **Photon and Electron Stimulated Desorption of Excimers from the Surface of Solid Neon**
T. Adachi(1), T. Hirayama(1), and I. Arakawa(1, 2); (1) *Gakushuin University*
(2) *Institute for Molecular Science, Okazaki*
12. **H⁺ Desorption and Hydrogen Pairing on the Hydrogenated Si(100) Surface**
S. Vijayalakshmia, H. T. Liub and Z. Wu, *Rutgers University- Newark*
13. **Electron Stimulated Desorption and Fragmentation of Physisorbed Ferrocene Studied by STM**
K. Svensson, T. R. Bedson and R. E. Palmer, *The University of Birmingham*
14. **New Close-Coupling Approach for Ion-Surface Interactions, Including Continuum Discretization**
B. Bahrim and U. Thumm, *Kansas State University*
15. **Electron Stimulated Dissociation of Ammonia on Ge(100)**
C. Bater, M. Sanders, J. H. Craig, Jr., *University of Texas*
16. **Electron-Beam Induced Damage of Molecular Solids Containing Polyatomic Anions**
N. G. Petrik, G. Teeter, M. T. Sieger and T. M. Orlando, *Pacific Northwest National Laboratory*
17. **"DIET" in the bulk: X-ray excitation of DX centers in AlGaAs**
Yeong-Ah Soh and G. Aepli *NEC Research Institute, E. D. Isaacs Lucent Technologies*, Frank M. Zimmermann, *Rutgers University*
18. **"Dissociative Adsorption and Recombinative Desorption of H₂ on Si(100): Solution of the "barrier puzzle""**, Frank M. Zimmermann and X. Pan, *Rutgers University*
19. **The Interaction of Low-Energy Molecular Ions with Surfaces**
Z. Marka, Y. Yao, B. Pratt-Ferguson, M. M. Albert, R. G. Albridge, G. L. Lüpke, A. Puckett, and N. H. Tolk, *Vanderbilt University*, G. Betz and W. Husinsky, *Technical University, Austria*, J. C. Tully, *Yale University*

1. Electron-Stimulated Desorption of Lithium Atoms from Oxidized Molybdenum Surfaces, V. N. Ageev (1), Yu. A. Kuznetsov (1), and T. E. Madey (2); (1) A. F. Ioffe Institute, (2) Rutgers University

We have measured electron-stimulated desorption (ESD) yields and energy distributions for lithium (Li) atoms from Li layers adsorbed at 300 K on an oxygen-monolayer-covered molybdenum surface as a function of electron energy and lithium coverage. The measurements have been carried out using a time-of-flight method and surface ionization detector. The appearance threshold for Li atoms is close to the oxygen 2s level ionization energy of 25 eV and is independent of the lithium coverage. The lithium atom ESD yield related to the threshold of 25 eV increases linearly with increasing lithium coverage. The additional threshold of 55 eV is observed in the lithium coverage range from 0 to 0.45. It may be associated with the lithium 1s level ionization energy. The lithium atom ESD yield related to the threshold of 55 eV passes through a maximum as the lithium coverage increases and decreases to zero at lithium coverages more than 0.45. The additional thresholds for lithium atoms at about 40 and 70 eV correlating with the ionization energies of the molybdenum 4p and 4s levels appear at the lithium coverages of 0.6 and 0.75, respectively. These thresholds have a view of sharp peaks indicating that desorption proceeds via a resonance process, in which the initial excitation may lead to a spectator electron in a quasi bound state.

The average kinetic energy of lithium atoms lies in the energy range of several tenths of eV. The ESD energy distribution for lithium atoms consists of a single peak with a maximum of around 0.18 eV at electron energies less than 55 eV. The second peak with a maximum of about 0.25 eV appears at electron energies more than 55 eV. As the lithium coverage increases the low-energy peak shifts toward low kinetic energies, while the high-energy peak decreases disappearing at lithium coverage 0.45. Simultaneously the Li atom energy distribution broadens toward low kinetic energies. The data can be interpreted by means of the Auger stimulated desorption model, in which neutralization of adsorbed lithium ions occurs after filling of holes created by incident electrons in inner shells of substrate and lithium atoms.

2. "Electron-Stimulated Desorption of Lithium Ions from Silicided Tantalum Surfaces", V. N. Ageev and S. M. Solovev, A. F. Ioffe Institute, St. Petersburg, Russia

Electron -stimulated desorption (ESD) of lithium ions has been studied from lithium layers adsorbed on silicided tantalum surfaces by means of a static magnetic mass spectrometer combined with a retarding field analyzer. The concentration of silicon in the subsurface region of a sample has been measured using Auger electron spectroscopy. The silicided tantalum surfaces is prepared by annealing at different temperatures silicon films deposited at room temperature onto the tantalum surface. The ESD appearance threshold for lithium ions is close to the lithium 1s level ionization energy of 55 eV and is independent of deposited lithium concentration. The additional thresholds are observed at about 130 and 150 eV. The 130 eV threshold exceeds by about 30 eV the ionization energy of the silicon 2p level and may be due to double ionization. The 150 eV threshold may be related to the ionization of silicon 2s level. The ESD yield of lithium ions are related to the 55 eV threshold and that are related to the 130 eV and 150 eV ones peak at different concentrations of deposited lithium.

There is no correlation between the maximum ESD yield of lithium ions and the concentration of silicon on the surface. This effect may be associated with the phase transitions in silicided tantalum occurring at different annealing temperatures. After heating the sample to higher than 1700K and cooling it to room temperature the ESD yield of lithium ions steeply increases. The main contribution to ion yield is due to additional thresholds. This high ESD yield of lithium ions may be connected with some unequilibrium sites of silicon atoms on the surface which are conserved after cooling it to room temperature. The concentration of these silicon atoms is too small to be detected by Auger electron spectroscopy. The results can be interpreted by the Auger stimulated desorption model taking into account the local surface field relaxation.

3. "ESD and PSD of Alkalies from Oxide Surfaces - Relevance to Tenuous Planetary Atmospheres", B. V. Yakshinskiy and Theodore E. Madey, *Rutgers University*

It is common belief that the Moon has no atmosphere. In fact, both the Moon and Mercury have tenuous atmospheres ($p < 1 \times 10^{-10}$ Torr) but neither can retain gaseous species for a considerable time; the atmospheric constituents must be continuously resupplied. To investigate mechanisms for the origin of Na and K in the atmospheres of the planet Mercury and the Moon [1, 2], we are studying the adsorption and desorption of Na deposited on model mineral surfaces: amorphous stoichiometric SiO_2 thin films, grown on a Re(0001) substrate at 300K. The adsorption-desorption of Na deposited onto these films have been investigated using x-ray photoelectron spectroscopy, low energy ion scattering, thermal desorption spectroscopy, electron- and photon-stimulated desorption (XPS, LEIS, TDS, ESD, and PSD). Na is found to grow on amorphous SiO_2 as a mostly ionic monolayer, followed by metallic island formation (Stranski-Krastonov growth mode). Fractional monolayers of Na desorb thermally in the temperature range 500-1000K, with desorption of multilayer Na at 350K. Na desorption is affected by ion bombardment, and by reaction with residual gases. ESD of Na^+ ions with average energy 2 eV is observed for incident electron energies above a threshold of 25 eV, corresponding to the $\text{O}2s$ excitation. We find that ESD of neutral Na occurs for electron energy thresholds as low as ~ 4 eV, that desorption cross sections are rather high ($\sim 1 \times 10^{-19} \text{ cm}^2$) at ~ 11 eV, and that desorbing atoms are "hot", with supra-thermal velocities (~ 0.1 eV). Moreover, photon-stimulated desorption of neutral Na occurs with a threshold energy of 4 eV, and the desorption cross section is $1 \times 10^{-20} \text{ cm}^2$ at 5 eV. We interpret the ESD/PSD of Na as occurring via a charge-transfer process, in which ionic Na^+ is converted to neutral Na, which desorbs. Whereas the ESD and PSD excitation processes are similar, the direct electron flux from the solar wind is too small to cause significant Na desorption; in contrast, the solar photon flux is large enough to maintain the observed Na lunar atmosphere. These data provide evidence that electronically-induced desorption mechanisms (e.g., PSD) may contribute as source processes for Na in tenuous planetary atmospheres. Where long-wavelength solar photons cause significant heating of the surface (e.g., 700K at Mercury's equator), thermal desorption can also contribute to the atmosphere.

[1] T. E. Madey, B. V. Yakshinskiy, V. N. Ageev, R. E. Johnson, *J. Geophys. Res. Planets* 103, 5873-5887 (1998).

[2] B. V. Yakshinskiy and T. E. Madey, *Nature* 400, 642-644 (1999).

4. "Low-Temperature Water Ice Phases Probed by Electron Stimulated Desorption", T. M. Orlando, M. T. Sieger and W. R. Wiley, *Pacific Northwest National Laboratory (PNNL)*

Low-energy electron-stimulated desorption (ESD) of D^+ from water has been used to examine the phase and growth behavior of nanoscale vapor-deposited ice films grown on Pt(111) between 90 - 155 K. The D^+ yield from porous amorphous solid water (deposited at 90 K) shows evidence for sintering near 120 K, increases between 120 - 140 K, and then drops at the amorphous-crystalline phase transition at 155 K. Ice deposited at 155 K forms an epitaxial crystalline film, with a D^+ yield nearly one-third larger than the yield from crystalline films prepared by annealing the amorphous phase. This suggests that the crystalline ordering or morphology of the annealed amorph is different than that of the epitaxial films. Ice deposited at 90 K on top of epitaxial crystalline ice is amorphous, but crystallizes to a form similar to that of an epitaxial film, suggesting that nucleation in this case proceeds from the buried interface. The studies demonstrate the utility of ESD to probe phase transitions of molecular solids, such as water.

5. "Electron-Induced Processes in Condensed Films of CF_2Cl_2 ", M. N. Hedhili (1), Q. B. Lu (1), T. E. Madey (1), M. Lachgar(2), Y. Le Coat(2), R. Azria(2), and M. Tronc(3); (1) *Rutgers University* (2) *Université Pierre et Marie Curie*, (3) *Université Paris-Sud*

We report measurements of electron stimulated desorption (ESD) yields and kinetic energy distributions of F^- and Cl^- from thin films of CF_2Cl_2 condensed on polycrystalline platinum. Dissociative electron attachment processes cause a peak in the F^- yield at an electron energy of ~ 4 eV and a peak in Cl^- yield at ~ 7 eV. The yields and kinetic energy distributions of Cl^- change as function of time during electron bombardment. These changes are attributed to the synthesis of Cl_2 in the condensed phase induced by electron bombardment of the CF_2Cl_2 film. Cl_2 formation is demonstrated by the observation after electron bombardment of the $2\Pi_u$ resonance in the Cl^- yield characteristic of condensed Cl_2 , and by Cl^- kinetic energy distributions which are similar to those obtained from condensed Cl_2 molecules.

6. "Photon Stimulated Ion Desorption of Poly-Methylmethacrylate and Poly-Isopropenylacetate Thin Films Following Oxygen Core Excitation"

K. Fujii**, S. Wada, D. Taga, Y. Nakashima, T. Sekitani and K. Tanaka, *Hiroshima University*, M. Tooyama, *Mitsubishi Rayon Co., Ltd., Otake, Japan*

Recent progress in synchrotron radiation (SR) techniques in the soft X-ray region has developed a new field in chemistry such as controlling chemical bond scission by a site-specific core electron excitation. Tinone et al. showed that site-specific ion desorption occurs in thin films of poly-methylmethacrylate (PMMA) by monochromatic soft X-ray excitation [1]. The efficient production of the CH_3^+ and CHO^+ ions was observed for the resonant core excitations of O_{1s} ($\text{OCH}_3 \rightarrow \sigma^*(\text{O}-\text{CH}_3)$) and $\text{O}_{1s}(\text{OCH}_3) \rightarrow \sigma^*(\text{C}-\text{OCH}_3)$, respectively. These studies indicate that the primary excitation directly contributes to the ion desorption from the specific site of the molecule. In the present work, poly-isopropenylacetate (PiPac) thin film was chosen as a sample. The monomer unit structure of PiPac is different in the position of the oxygen comparing to the PMMA. In order to reveal the effect of the difference in functional group to ion desorption, we have studied the photon stimulated ion desorption for these polymer thin films following oxygen core electron excitation.

Thin films of polymers were prepared by spin casting on Au-evaporated Si(100) wafers from methyl ethyl ketone solutions. The thickness of the films was estimated to be less than 200 Å. Experiments were performed at the soft X-ray beamline BL11A of Photon Factory (KEK-PF). Desorbing ions were detected using a time-of-flight mass spectrometer with a pulsed SR^2 . TOF Åfs of the ions were measured as the time difference between the SR pulse and the signals which were detected through the 9 cm drift tube.

H^+ , CH^+ , CH_2^+ , CH_3^+ and CHO^+ ions are mainly desorbed from PMMA thin films following oxygen core excitation, while H^+ , CH^+ , CH_2^+ , CH_3^+ and COCH_3^+ are from PiPac. Four common features are seen in both total electron yield spectrum and partial ion yield spectra of the main ions. The remarkable difference is observed in the ion yield of PiPac between the CH_3^+ and the COCH_3^+ ions. Tinone et al. have shown that the detection of ions has an advantage over total electron detection, namely, more clear differentiation and assignment of transitions from different atomic sites by considering the connection of the fragment ion to the original molecule. The enhancement of CH_3^+ ions suggests that this primary excitation related to the anti-bonding orbital localized in the C- CH_3 bond, while the enhancement of COCH_3^+ ions suggests the anti-bonding orbital localized in the O- COCH_3 bond.

[1] M. C. K. Tinone, K. Tanaka, J. Maruyama, N. Ueno, M. Imamura and N. Matsubayashi, *J. Chem. Phys.*, **100**, 5988 (1994).

[2] K. Tanaka, M. C. K. Tinone, H. Ikeura, T. Sekiguchi and T. Sekitani, *Rev. Sci. Instr.*, **66**, 1474 (1995).

** Competing for Student Award

7. "A Study of Photon Induced Processes with Adsorption-Desorption of Glycine at the $\text{TiO}_2(110) (1 \times 2)$ Surface", E. Soria(1), I. Inmaculada(2), E. Roman(3), E.M. Williams(4), and J.L. de Segovia(1); (1) CETEF "L. Torres Quevedo" (2) *Universidad Carlos III*, (3) *CSIC*, (4) *The University of Liverpool*

Processes of adsorption-desorption with glycine admitted to the $\text{TiO}_2 (110) (1 \times 2)$ reconstructed surface have been studied using synchrotron light in the energy range 35 -110 eV. Glycine was admitted to attain initially multilayer proportions (~ 2 ML) at the surface at room temperature and the desorption to mono and sub-monolayer scale was followed with both thermal desorption and desorption induced by the photon flux. At the initial clean surface, the photoelectron spectrum shows the presence of Ti 3d electrons, but without any associated Ti^{3+} character in the Ti 3p spectrum. Desorption under photon irradiation of glycine multilayers is seen to bring about an enhancement of the latter Ti^{3+} form, which is not feature with thermal desorption (temperature range up to 160 C). In the experiments, altogether the C (2s), N(2s) and O(2s) related to glycine are also monitored and it is observed that the N(2s) feature undergoes a change ~ 0.5 eV in energy position in the region of one monolayer. The desorption cross-sections of the adsorbate are generally large ($< 10^{-16} \text{ cm}^2$).

To gain insight of the processes involved with these desorption phenomena as well as the bonding configurations, we have studied the response of the surface during adsorption of glycine at the clean (1×2) surface. There is evidence of an immediate attenuation of the intensity of the Ti 3d which proceeds in parallel with the concomitant growth of the C(2s) derived from the adsorbate. These actions appear ahead of the build of the main features of glycine adsorption, as reflected in the growth of the N(2s) and O(2s)/glycine features, and the strong attenuation of the O(2s)/substrate signal. The indications are, thus, of a dissociation process at the sub-monolayer scale. It is interesting to note that when desorbing multilayers either thermally or by photon induced desorption, the surface at the monolayer stage shows a different near-valence spectrum, reinforcing the distinction between mono and multilayer regimes.

We are currently complementing our observations at the synchrotron by ESD studies in our laboratory in which the species of desorbed ions and their associated energy characteristics will be followed with some interest. The study is aimed particularly with a view to examine i) the transition from multi to mono/sub-mono glycine coverage, and ii) the initial stages of glycine adsorption at the clean surface.

8. "Time-Of-Flight Techniques for the Investigation of Kinetic Energy Distributions of Ions and Neutrals Desorbed by Core Excitations", R. Weimar(1), R. Romberg(1), S. Frigo(2), B. Kassuehlke(1); and P. Feulner(1); (1) *Technische Universität München*, (2) *Advanced Photon Source, Argonne*

In gas phase core level photodissociation experiments, the determination of kinetic energies (KE) of photoions from their time of flight (TOF) in the detector is a standard technique which yields valuable information on the microscopic reaction details. On surfaces, and particularly for strongly coupled chemisorbates on metals, the experimental situation is more difficult, because of rapid charge transfer (effectively shifting intensity from ionic to neutral desorption channels) and recapture. In the near threshold region, PSD of ions may be quenched completely whereas desorption of neutrals (molecules and fragments) still persists. Analytical tools are therefore required which yield KE distributions for ions *and* neutrals, in particular if the cross-over from mainly neutral (for one hole excitations) to mainly ionic PSD (multiple hole excitations) is of interest. They have to be highly sensitive because of the small core level excitation cross sections, and the limited photon flux that is available for narrow band excitation.

We have designed simple KE detectors for ions and neutrals based on mass spectrometers and TOF techniques, and demonstrate their performances by KE data on charged and neutral CO and O particles desorbed from chemisorbed CO/Ru(001). To the best of our knowledge, our data are the first example of any KE distribution of neutral core-hole induced PSD, in particular of neutral fragments. The ion detector consists of a linear TOF mass spectrometer which is operated at BESSY during single bunch runs. We derive the masses of desorbing particles from the center of gravity of their TOF peaks, and their KE distributions from the shapes of the peaks. This approach is very efficient because all masses and KEs are monitored simultaneously. For neutrals we use post-ionization by pulsed electron impact and mass separation in a quadrupole filter, and evaluate the KE from the flight time through the filter. The method is particularly well suited for energetic particles like molecular fragments, where the application of mechanical choppers is difficult. Applied to PSD of O atoms from CO/Ru(001) by O1s excitation, we find clearly different KE distributions with centers of gravity shifting from 1 to 2.7 eV when going from the sub-threshold region to the π^* -resonance (1h-1e), and to the [O1s, 1π] $2\pi^2$ (2h-2e) excitation. The O⁺ energies, on the other hand, exhibit non-monotonic behavior. They are maximal at the π -resonance (8.4 eV), go through a minimum at the 2h-2e state (4.1 eV) and increase again for a 3h-3e state (6.5 eV) and in the multiple shake-off regime. Mechanisms and possible contributions of ultrafast processes are discussed.

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9. "PSD of Neutral Hydrogen Atoms from Condensed Water and Ammonia by Resonant O1s and N1s Excitation: Search for the Signature of Ultrafast Bond Breaking", R. Romberg, S. Frigo(1), A. Ogurtsov(2), P. Feulner, and D. Menzel, *Technische Universität München*, (1) *Advanced Photon Source* (2) *Verkin Institute for Low Temperature Physics & Engineering, Kharkov, Ukraine***

Ultrafast dissociation and desorption (UFD), e.g. breaking of the bond during the lifetime of the core hole, is an intensely studied topic since first evidence appeared in electron spectroscopy (Morin and Nenner, PRL **56**, 1913) and photon stimulated desorption (Coulman et al., Chem. Phys. Lett. **148**, 371). Optimum candidates for the investigation of these processes are systems which exhibit i) highly repulsive core-excited states, ii) at least one light reaction partner that is quickly accelerated and considerably displaced from its ground state equilibrium position before core hole decay, and iii) a not too short-lived core hole. Water should be well suited because the lowest neutral O1s excitation is clearly antibonding (it appears as a broad peak in the photoabsorption of the isolated molecule without any vibrational fine structure), and because previous PSD experiments yielded enhanced H^+ -PSD for these resonances which has been explained in terms of UFD. However, if UFD were completed before dissociation, and charge transfer reactions after core decay were negligible, emission of neutral H atoms and not of ions should occur, which is in some contradiction to the previous findings. The goal of the present experiments was to increase the sensitivity of an existing detector for neutral particles (S. Frigo et al., PRL **80**, 2813) such that detection of neutral H atoms becomes possible, and to compare H and H^+ -PSD for resonant 1s excitation for water and also for ammonia, which in previous PSD-experiments showed similar H^+ enhancement as water.

An increase of the detector's sensitivity that was sufficient for the investigation of hydrogen atoms was maintained by a reduced background pressure due to more effective pumping of the detector volume. Multilayers of water and ammonia, and bilayers of water have been investigated. The previous results on photoabsorption and ion PSD have been reproduced (with better spectral resolution) for all systems in every detail, in particular the strong enhancement of H^+ -emission in the threshold region. We also find that H_2^+ PSD is enhanced for the threshold resonances, although less strongly than H^+ , and discuss alternative explanations for this result. For neutral H atoms, however, no enhancement exists at the threshold resonances, for water as well as for ammonia. This surprising result indicates that post-core decay charge transfer processes between the reaction products *are* important for our systems even though UFD-contributions certainly exist. It shows in particular that judging UFD-contributions from the relative abundances of charged fragments without a detailed study of post-decay charge transfer is a rather unreliable approach.

Supported by the Deutsche Forschungsgemeinschaft (Me 266/21-1; 2).

**Competing for Student Award

10. "A New Analyser for Gas and Ion Analysis: The SPLAT Analyser", Robert G. Jones and N.E. Abrams, *University of Nottingham*

We describe a general purpose analyser for ions and gases, capable of measuring the velocity (speed and direction) as an image for any particular mass and internal rovibrational state (for state specific ionisation). A prototype of the device, called the S^{PEED} by L^{INEAR} A^{NALYSIS} of T^{RAJECTORY} (SPLAT) analyser has been built and tested using integral electron beam ionisation (for ion analysis, no internal ionisation source is required). Gas (or ions from a pulsed source) enter the device through an aperture, beyond which a narrow, pulsed ($<1\ \mu\text{s}$), electron beam (or laser beam), ionises it to form a line of ions. The parent molecular ions continue to move with the same velocity as the neutral molecules from which they originated, the velocity vectors forming a flat pancake in which all the vectors project back to the aperture. After a time delay (10-100's μs) the parent ions disperse such that the pancake of ions is a polar distribution of speed versus angle. A repeller plate is then pulsed on and the pancake of ions is accelerated perpendicularly to its original motion [1] and transported, via a novel ion optic system with spatial and temporal focussing, to a channelplate/fluorescent screen/CCD camera assembly. During this second flight time the ions disperse into a series of pancakes of different masses, any one of which can be viewed by pulsing on the channelplate after the second delay time (0 - 10 μs). The advantages of this device are:

- (i) Analysis at very low (thermal) energies (10 - 100's of meV).
- (ii) Velocity measured directly within a single plane, no assumptions needed to extract the distributions.
- (iii) Can be configured to analyse gas or ions from extended sources, beams, or point sources.

The performance of this analyser is assessed in terms of speed, angle and mass resolution using bulk gas and molecular beams.

[1] D. Corr and D.C. Jacobs, *Rev. Sci. Instrum.* **63** (1992) 1969

11. "Photon and Electron Stimulated Desorption of Excimers from the Surface of Solid Neon", T. Adachi(1), T. Hirayama(1), and I. Arakawa(1, 2); (1) Gakushuin University, (2) Institute for Molecular Science, Okazaki

We have been studying the desorption of excited particles from the surface of rare gas solids (RGSs) induced by exciton creation using photon- and electron-stimulated desorption (PSD and ESD) techniques.[1] As to the excited atom desorption, two mechanisms, excimer dissociation (ED) and cavity ejection (CE), have been proposed and confirmed experimentally. Desorption of an excimer from the surface of RGSs has been predicted theoretically for solid Ne, Ar, and Kr, but the experimental evidence has been obtained only for solid Ar[2]. In the present study we have confirmed the desorption of $\text{Ne}_2^* \ ^3\Sigma_u$ from the surface of solid Ne induced by the surface and bulk excitons using low energy electron and monochromatic VUV radiation as excitation sources.

PSD and ESD experiments have been done at the beam line BL5B in UVSOR (Institute for Molecular Science, Okazaki), and at Gakushuin University, respectively. The experimental setup is similar to the one used in our previous work[1] equipped with a pin hole camera in order to observe the spatial distribution of the emitted light. Emission lifetime of the desorbed excited particles has been estimated by measuring decay curves using a pulsed electron beam.

In 2-dimensional spatial distribution of the emission, we have observed a "plume" clearly apart from the sample surface, indicating the emission from the desorbed excited particles. By measuring the decay curves of the emission, the lifetime was estimated to be in the order of 10^{-6} s, which is consistent with the radiative lifetime of $\text{Ne}_2^* \ (^3\Sigma_u)$ in gas phase. Detailed analysis of the decay curve shows that the desorbed excimer initiated by a creation of a surface exciton is in highest vibrational state. This can be understood if we consider the fast desorption process via CE mechanism ($\sim 10^{-11}$ s [4]) and slow vibrational relaxation in solid Ne ($>10^{-7}$ s [5]). Estimated kinetic energy of desorbed Ne_2^* (0.2 ± 0.1 eV) also supports the CE mechanism for excimer desorption.

[1] I. Arakawa, Molecular Crystals and Liquid Crystals (Gordon and Breach Science Publishers, New York, 1998), Vol.314, p47, and references therein.

[2] C. Reimann et al., Phys. Rev. B **37**, 1455 (1988).

[3] E.V. Savchenko et al., Surf. Sci. **390** 261 (1997).

[4] L.F. Chen et al., Nucl. Instrum. Meth. Phys. Res. B **116**, 61 (1996).

[5] F. Coletti et al., J. Chem. Phys. **83**, 49 (1985).

12. "H⁺ Desorption and Hydrogen Pairing on the Hydrogenated Si(100) Surface",
S. Vijayalakshmia, H. T. Liub and Z. Wu, *Rutgers, University - Newark*

We report desorption of H⁺ ions from hydrogenated Si(100) surface under the irradiation of low fluence 193 nm pulsed laser beam. The kinetic energy of the H⁺ ions are measured using time-of-flight (TOF) technique. Monohydride and dihydride surfaces show little differences. We observed two groups of H⁺ ions with mean kinetic energies of 0.09 ± 0.05 eV and 0.38 ± 0.06 eV, respectively, without taking into account the correction due to image interaction. The ratio of the 0.38 eV peak to the 0.09 eV peak increased with the substrate temperature. The experimental results are interpreted using the hydrogen pairing model on Si(100). The 0.09 eV peak and the 0.38 eV peak are assumed to correspond, respectively, to the H⁺ ions desorbing from doubly occupied and singly occupied dimers. The difference of 0.29 ± 0.11 eV in the kinetic energies of these two groups of H⁺ ions is compared with the pairing energy on the H/Si(100) surface. The kinetic energy of the H⁺ ions also provides an estimate of the hole-hole repulsion energy in the Si-H bond. The estimated value of 9.4 eV agrees with earlier experimental results.

13. "Electron Stimulated Desorption and Fragmentation of Physisorbed Ferrocene Studied by STM", K. Svensson, T. R. Bedson and R. E. Palmer, *The University of Birmingham*

Ferrocene (C_5H_5)₂Fe is an organic metal with the potential to be used for deposition of iron into predetermined patterns on surfaces. Control of the dissociation process may lead to a reliable method of device fabrication on the nanometer scale. We have used high resolution electron energy loss spectroscopy and scanning tunnelling microscopy to study the influence of electron impact on ferrocene adsorbed on graphite (HOPG). Ferrocene physisorbs on HOPG and displays a vibrational spectrum similar to the gas phase molecule; from the mode assignment we conclude that ferrocene adsorbs with one of the 5-fold rings parallel to the surface. The influence of electron impact on this system can be separated into three energy regimes. For low electron energies (< 10 eV), where the molecule shows a negative ion resonance state in the gas phase the ferrocene molecules were preferentially desorbed. At intermediate electron energies (20-100 eV) partial fragmentation of the ferrocene molecules occur, while at higher electron energies (>200 eV) more complete dissociation takes place leaving nanometre-scale clusters, presumably composed of iron, on the surface. Analogies are drawn with photon, thermal and very high energy electron induced dissociation and desorption.

14. "New Close-Coupling Approach for Ion-Surface Interactions, Including Continuum Discretization", B. Bahrim and U. Thumm, *Kansas State University*

Within a two-center close-coupling expansion, we rewrite the time-dependent Schrödinger equation for an active electron interacting with a slow moving projectile and a metal surface, as a system of coupled differential equations and solve this system numerically. In contrast to other close-coupling approaches (e.g. ref. ¹), we fully discretize the active electrons motion inside the metal, by using a discrete sum of Weyl ² wave packets, instead of a continuum of jellium wave functions. In particular, these transfer processes are of relevance to the population evolution of desorbed ions and atoms. For the H/Al system, we provide level shifts, transition rates for atom-metal transitions, the time evolution of the atomic and metallic population amplitudes (including systematic convergence studies with respect to the number of atomic and metallic basis states), and excitation rates for one-electron transitions in the substrate.

[†]Work supported by NSF under grant PHY-9604872 and the Division of Chemical Sciences, Office of Basic Energy Sciences, Office of Energy Research, U.S. DOE.

¹ P. Kürpick, U. Thumm and U. Wille, Phys. Rev. A 56, 543 (1997); P. Kürpick and U. Thumm, Phys. Rev. A 58, 2174 (1998)

² G. Schiwietz, Phys. Rev. A 42, 296 (1990)

15. "Electron Stimulated Dissociation of Ammonia on Ge(100)", C. Bate, M. Sanders, J. H. Craig, Jr., *University of Texas*

Electron stimulated dissociation of adsorbed ammonia on Ge(100) at 100K was studied using electron stimulated desorption (ESD), X-ray photoelectron spectroscopy (XPS), and high resolution electron energy loss spectroscopy (HREELS). Electron induced dissociation and nitridation of the Si(100) surface using ammonia as a precursor has been extensively explored in our laboratory. Since Ge(100) exhibits the same (2x1) reconstruction as does Si(100), we have initiated studies to determine whether this similarity extends to germanium nitride formation stimulated by low energy electron irradiation. XPS studies of binding energy changes associated with the N 1s state will be presented resulting from electron irradiation of adsorbed ammonia. HREELS data will also be presented showing the characteristic vibrational spectra of adsorbed ammonia on Ge(100) at 100K and the dissociation products resulting from electron irradiation. Time of flight distributions of H^+ will be presented resulting from electron desorption from both germanium hydride and adsorbed ammonia.

16. "Electron-Beam Induced Damage of Molecular Solids Containing Polyatomic Anions", N. G. Petrik, G. Teeter, M. T. Sieger and T. M. Orlando, Pacific Northwest National Laboratory

Electron-stimulated desorption (ESD) of anhydrous single crystals of NaNO_3 as well as hydrated and dehydrated granular samples of MgSO_4 , Na_2CO_3 and Na_2SO_3 have been examined using quadrupole mass spectrometry and post-irradiation temperature programmed desorption. The ESD cross section due to irradiation of NaNO_3 single crystals with 100 eV electrons is at least 10^{-16} cm^2 . This large cross section is primarily due to the efficient damage of the singly-charged nitrate groups. In contrast, the damage cross section in all other salts (both hydrated and dehydrated) studied is considerably lower and approaches our detection limits of about 10^{-21} cm^2 . The ESD mechanisms and reasons for the relative stabilities of these complicated salts will be addressed.

17. **""DIET"" in the bulk: X-ray excitation of DX centers in AlGaAs**", Yeong-Ah Soh and G. Aeppli, *NEC Research Institute*, E. D. Isaacs, *Lucent Technologies*, Frank M. Zimmermann, *Rutgers University*

Si dopants in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ act as deep donor levels (DX centers) when $x > 0.22$. These DX centers can be photoexcited to a metastable state in which they are shallow donors. In analogy to DIET processes at surfaces, the excitation process involves atomic motion on an excited-state potential energy surface, resulting in a drastic atomic rearrangement in the bulk. In addition to the structural change, two electrons are injected into the conduction band in the process, increasing the conductivity. In this work, we report on the first-time use of X-rays to excite DX centers into their shallow donor state, monitored by measuring the resulting persistent photoconductivity. The energy dependence of the photoconductivity closely follows the simultaneously detected X-ray fluorescence, indicating that photoexcitation of core holes is an efficient primary excitation step for the excitation of DX centers. However, there is no appreciable difference between the Ga and As K-edges, implying a non-local DX center excitation mechanism. We verified that this non-locality extends to macroscopic length scales by monitoring the photoconductance of a macroscopic sample excited by an X-ray microbeam.

18. "Dissociative Adsorption and Recombinative Desorption of H₂ on Si(100): Solution of the "Barrier Puzzle"", Frank M. Zimmermann and X. Pan, *Rutgers University*

The interaction of hydrogen with Si(100) is of considerable technological importance since hydrogen desorption is the rate-limiting step in the low-temperature chemical vapor deposition of Si. Furthermore, this system is intriguing from a fundamental point of view, due to a multitude of unusual and remarkable experimental observations, such as desorption kinetics intermediate between first order and second order, and the so-called "barrier puzzle": A large barrier to adsorption is seen in adsorption experiments, whereas in desorption dynamics experiments the desorbing molecules paradoxically show no signs of having traversed such a barrier.

Using surface second harmonic generation, we have measured the adsorption and desorption kinetics as a function of surface temperature, H coverage, and exposure pressure. These measurements reveal more highly unusual kinetic behavior. Contrary to what is expected from Langmuirian site-blocking considerations, the sticking probability increases markedly with coverage, indicating a self-catalyzed adsorption mechanism. In addition, the sticking probability exhibits a pronounced dependence on exposure pressure, ruling out most "simple" adsorption mechanisms. The observations are interpreted in terms of an autocatalytic, barrier-less, inter-dimer adsorption mechanism (observed with the STM by Biedermann et al., submitted). Our model quantitatively explains the measured adsorption and desorption kinetics (temperature, coverage, and pressure dependence), and provides a natural explanation of the vexing barrier puzzle. Fitted model parameters are in very good agreement with independently obtained experimental and theoretical values.

19. "The Interaction of Low-Energy Molecular Ions with Surfaces", Z. Marka, Y. Yao, B. Pratt-Ferguson, M. Albert, R. G. Albridge, G. Luepke, A. Puckett, and N. H. Tolk, *Vanderbilt University*

An experimental evidence is presented for a new nonlinear effect in the sputtering yields of molecular ions at near-threshold energies. We measured the sputtering yield in a polycrystalline gold sample for several different molecular (N_2^+ , O_2^+ , NO, CO) and atomic projectiles. When the yields for the molecular projectiles are compared to the yields for the constituent atoms at the same projectile velocity, a pronounced enhancement is observed at near-threshold energies. We attribute this effect to enhanced energy transfer to the surface by an incident diatomic molecule compared to energy transferred by two incident uncorrelated atoms. The onset of the effect, which increases with decreasing energy, is different for each studied molecule and it follows the order of their vibrational periods but not their bond strength. We argue, that the comparison of the collision time to the vibration time of the molecule determines when molecular enhancement can be observed.

Recent molecular dynamics (MD) simulations reproduce an increased sputtering yield of N_2 molecule at low energies. These calculations show that the two key factors for the onset of this effect are: (1) the molecular potential (determines vibrational time) and (2) the molecule-surface interaction potential (determines the collision time). Variation of these potentials in our MD calculations provide a strong evidence that the comparison of these two timescales determines when this new effect can be observed. The calculation of an exact gold- N_2 potential is under way.

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